Figure 1

Table 1. Crystallographic data and refinement statistics

	Native data set
Wavelength (Å)	1.0526
Resolution range (Å)[1]	50.0-2.0 (2.07-2.0)
No. of observed reflections	164,206
No. of unique reflections	27,881
No. of reflections in R_{free} set	828
Completeness (%)	99.2(99.4)
$I/\sigma(I)$	19.6(1.4)
(R_{merge}) (%)[2]	3.9(20.9)
R_{cryst}/R_{free} (%)[3]	21.8/23.8
No. of refined non-hydrogen atoms[4]	
protein	2248
water	265
Average B-factor (all atoms, Å^2)	60
Wilson B-factor (Å^2)	45
R.m.s. Δ bond lengths/angles[5]	0.0081/1.7
Residues in allowed regions (%)[6]	97%

[1]Values in parentheses are statistics for the highest resolution bin.

[2]$R_{merge}\ (I) = \sum_{hkl}|Ihkl - <Ihkl>| / \sum_{hkl} Ihkl$, where $Ihkl$ is the measured intensity of the reflections with indices hkl.

[3]$R = \sum_{hkl}||Fo| - |Fc|| / \sum |Fo|$, where $|Fo|$ and $|Fc|$ are the observed and calculated structure factor amplitudes for reflection hkl, applied to the work (R_{cryst}=97%) and test (R_{free}=3%) sets, respectively.

[4]Residues -2, 239 and 240 were not located. Residues originating from the cloning site were given negative integers.

[5]Root mean squared deviations (rms Δ) in bond length and angles from ideal values.

[6]The Ramachandran plot was calculated according to Kleywegt and Jones, (1996).

Figure 2 (Table 2 (page 1))

```
HEADER      CELL ADHESION                                   1QZ1
TITLE       CRYSTAL STRUCTURE OF THE IG 1-2-3 FRAGMENT OF NCAM
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: NEURAL CELL ADHESION MOLECULE 1, 140 KDA ISOFORM;
COMPND      3 CHAIN: A;
COMPND      4 FRAGMENT: IG MODULES 1-2-3;
COMPND      5 SYNONYM: N-CAM 140, NCAM-140;
COMPND      6 ENGINEERED: YES
SOURCE      MOL_ID: 1;
SOURCE      2 ORGANISM_SCIENTIFIC: RATTUS NORVEGICUS;
SOURCE      3 ORGANISM_COMMON: RAT;
SOURCE      4 GENE: NCAM1;
SOURCE      5 EXPRESSION_SYSTEM: PICHIA PASTORIS;
SOURCE      6 EXPRESSION_SYSTEM_COMMON: FUNGUS;
SOURCE      7 EXPRESSION_SYSTEM_STRAIN: GS-115;
SOURCE      8 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE      9 EXPRESSION_SYSTEM_PLASMID: PHIL-S1
KEYWDS      IG MODULES, CELL ADHESION, NCAM
EXPDTA      X-RAY DIFFRACTION
AUTHOR      V.SOROKA, K.KOLKOVA, J.S.KASTRUP, K.DIEDERICHS, J.BREED,
AUTHOR      2 V.V.KISELYOV, F.M.POULSEN, I.LARSEN, W.WELTE, V.BEREZIN,
AUTHOR      3 E.BOCK, C.KASPER
JRNL        AUTH   V.SOROKA, K.KOLKOVA, J.S.KASTRUP, K.DIEDERICHS,
JRNL        AUTH 2 J.BREED, V.V. KISELYOV, F.M.POULSEN, I.LARSEN,
JRNL        AUTH 3 W.WELTE, V.BEREZIN, E.BOCK, C.KASPER
JRNL        TITL   STRUCTURE AND INTERACTIONS OF NCAM IG1-2-3 SUGGEST
JRNL        TITL 2 A NOVEL ZIPPER MECHANISM FOR HOMOPHILIC ADHESION
JRNL        REF    TO BE PUBLISHED
JRNL        REFN
REMARK   1
REMARK   1 REFERENCE 1
REMARK   1   AUTH   C.KASPER,H.RASMUSSEN,J.S.KASTRUP,S.IKEMIZU,
REMARK   1   AUTH 2 E.Y.JONES,V.BEREZIN,E.BOCK,I.K.LARSEN
REMARK   1   TITL   STRUCTURAL BASIS OF CELL-CELL ADHESION BY NCAM
REMARK   1   REF    NAT.STRUCT.BIOL.               V.   7   389 2000
REMARK   1   REFN   ASTM NSBIEW  US ISSN 1072-8368
REMARK   1 REFERENCE 2
REMARK   1   AUTH   C.KASPER,H.RASMUSSEN,V.BEREZIN,E.BOCK,I.K.LARSEN
REMARK   1   TITL   EXPRESSION, CRYSTALLIZATION AND PRELIMINARY X-RAY
REMARK   1   TITL 2 ANALYSIS OF THE TWO AMINO-TERMINAL IG DOMAINS OF
REMARK   1   TITL 3 THE NEURAL CELL ADHESION MOLECULE (NCAM)
REMARK   1   REF    ACTA CRYSTALLOGR., SECT.D     V.  55   1598 1999
REMARK   1   REFN   ASTM ABCRE6  DK ISSN 0907-4449
REMARK   2
REMARK   2 RESOLUTION. 2.00 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM      : CNS 1.0
REMARK   3   AUTHORS      : BRUNGER,ADAMS,CLORE,DELANO,GROS,GROSSE-
REMARK   3                : KUNSTLEVE,JIANG,KUSZEWSKI,NILGES, PANNU,
REMARK   3                : READ,RICE,SIMONSON,WARREN
REMARK   3
REMARK   3   REFINEMENT TARGET : ENGH & HUBER
REMARK   3
REMARK   3   DATA USED IN REFINEMENT.
REMARK   3    RESOLUTION RANGE HIGH (ANGSTROMS) : 2.00
REMARK   3    RESOLUTION RANGE LOW  (ANGSTROMS) : 48.64
```

Figure 2 (Table 2 (page 2))

```
REMARK   3   DATA CUTOFF                  (SIGMA(F)) : 0.000
REMARK   3   DATA CUTOFF HIGH            (ABS(F)) : NULL
REMARK   3   DATA CUTOFF LOW             (ABS(F)) : NULL
REMARK   3   COMPLETENESS (WORKING+TEST)    (%) : 99.2
REMARK   3   NUMBER OF REFLECTIONS             : 28289
REMARK   3
REMARK   3   FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD         : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION  : RANDOM
REMARK   3   R VALUE            (WORKING SET) : 0.218
REMARK   3   FREE R VALUE                     : 0.238
REMARK   3   FREE R VALUE TEST SET SIZE   (%) : NULL
REMARK   3   FREE R VALUE TEST SET COUNT      : 828
REMARK   3   ESTIMATED ERROR OF FREE R VALUE  : NULL
REMARK   3
REMARK   3   FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED           : NULL
REMARK   3   BIN RESOLUTION RANGE HIGH       (A) : 2.00
REMARK   3   BIN RESOLUTION RANGE LOW        (A) : 2.13
REMARK   3   BIN COMPLETENESS (WORKING+TEST) (%) : 99.00
REMARK   3   REFLECTIONS IN BIN    (WORKING SET) : NULL
REMARK   3   BIN R VALUE           (WORKING SET) : 0.3730
REMARK   3   BIN FREE R VALUE                    : 0.4390
REMARK   3   BIN FREE R VALUE TEST SET SIZE  (%) : NULL
REMARK   3   BIN FREE R VALUE TEST SET COUNT     : 148
REMARK   3   ESTIMATED ERROR OF BIN FREE R VALUE : 0.036
REMARK   3
REMARK   3   NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   PROTEIN ATOMS          : 2247
REMARK   3   NUCLEIC ACID ATOMS     : 0
REMARK   3   HETEROGEN ATOMS        : 0
REMARK   3   SOLVENT ATOMS          : 265
REMARK   3
REMARK   3   B VALUES.
REMARK   3   FROM WILSON PLOT          (A**2) : 42.00
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : 60.60
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) : 7.90000
REMARK   3    B22 (A**2) : -15.20000
REMARK   3    B33 (A**2) : 7.30000
REMARK   3    B12 (A**2) : 0.00000
REMARK   3    B13 (A**2) : 0.00000
REMARK   3    B23 (A**2) : 0.00000
REMARK   3
REMARK   3   ESTIMATED COORDINATE ERROR.
REMARK   3    ESD FROM LUZZATI PLOT        (A) : 0.30
REMARK   3    ESD FROM SIGMAA              (A) : 0.36
REMARK   3    LOW RESOLUTION CUTOFF        (A) : 5.00
REMARK   3
REMARK   3   CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK   3    ESD FROM C-V LUZZATI PLOT    (A) : 0.35
REMARK   3    ESD FROM C-V SIGMAA          (A) : 0.42
REMARK   3
REMARK   3   RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3    BOND LENGTHS                 (A) : 0.008
REMARK   3    BOND ANGLES            (DEGREES) : 1.70
REMARK   3    DIHEDRAL ANGLES        (DEGREES) : 27.50
```

Figure 2 (Table 2 (page 3))

```
REMARK    3    IMPROPER ANGLES            (DEGREES) : 0.95
REMARK    3
REMARK    3    ISOTROPIC THERMAL MODEL : ANISOTROPIC
REMARK    3
REMARK    3    ISOTROPIC THERMAL FACTOR RESTRAINTS.    RMS      SIGMA
REMARK    3     MAIN-CHAIN BOND                 (A**2) : NULL  ; NULL
REMARK    3     MAIN-CHAIN ANGLE                (A**2) : NULL  ; NULL
REMARK    3     SIDE-CHAIN BOND                 (A**2) : NULL  ; NULL
REMARK    3     SIDE-CHAIN ANGLE                (A**2) : NULL  ; NULL
REMARK    3
REMARK    3    BULK SOLVENT MODELING.
REMARK    3     METHOD USED : NULL
REMARK    3     KSOL        : NULL
REMARK    3     BSOL        : NULL
REMARK    3
REMARK    3    NCS MODEL : NULL
REMARK    3
REMARK    3    NCS RESTRAINTS.                         RMS    SIGMA/WEIGHT
REMARK    3     GROUP  1   POSITIONAL            (A) : NULL  ; NULL
REMARK    3     GROUP  1   B-FACTOR           (A**2) : NULL  ; NULL
REMARK    3
REMARK    3    PARAMETER FILE  1   : NULL
REMARK    3    TOPOLOGY FILE   1   : NULL
REMARK    3
REMARK    3    OTHER REFINEMENT REMARKS: RESIDUES 241-242 WERE NOT LOCATED IN
REMARK    3    THE ELECTRON DENSITY MAP
REMARK    4
REMARK    4 1QZ1 COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK  100
REMARK  100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 17-SEP-2003.
REMARK  100 THE RCSB ID CODE IS RCSB020242.
REMARK  200
REMARK  200 EXPERIMENTAL DETAILS
REMARK  200    EXPERIMENT TYPE                 : X-RAY DIFFRACTION
REMARK  200    DATE OF DATA COLLECTION         : 06-NOV-2000; 04-DEC-2000
REMARK  200    TEMPERATURE          (KELVIN) : 100.0
REMARK  200    PH                              : 5.20
REMARK  200    NUMBER OF CRYSTALS USED         : 1
REMARK  200
REMARK  200    SYNCHROTRON             (Y/N) : Y; N
REMARK  200    RADIATION SOURCE                : MAX II ; ROTATING ANODE
REMARK  200    BEAMLINE                        : I711
REMARK  200    X-RAY GENERATOR MODEL           : NULL; HOME SOURCE
REMARK  200    MONOCHROMATIC OR LAUE   (M/L) : M
REMARK  200    WAVELENGTH OR RANGE       (A) : 1.0526; 1.54
REMARK  200    MONOCHROMATOR                   : NULL
REMARK  200    OPTICS                          : NULL
REMARK  200
REMARK  200    DETECTOR TYPE                   : IMAGE PLATE; IMAGE PLATE
REMARK  200    DETECTOR MANUFACTURER           : MARRESEARCH; MARRESEARCH
REMARK  200    INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK  200    DATA SCALING SOFTWARE           : SCALEPACK
REMARK  200
REMARK  200    NUMBER OF UNIQUE REFLECTIONS  : 27881
REMARK  200    RESOLUTION RANGE HIGH     (A) : 2.000
REMARK  200    RESOLUTION RANGE LOW      (A) : 50.000
REMARK  200    REJECTION CRITERIA  (SIGMA(I)) : 0.000
```

Figure 2 (Table 2 (page 4))

```
REMARK 200
REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE     (%)  : 99.2
REMARK 200  DATA REDUNDANCY                  : 5.900
REMARK 200  R MERGE                   (I)  : 0.03900
REMARK 200  R SYM                     (I)  : 0.03900
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET   : 19.6000
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.00
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 2.07
REMARK 200  COMPLETENESS FOR SHELL    (%)  : 99.4
REMARK 200  DATA REDUNDANCY IN SHELL        : 3.80
REMARK 200  R MERGE FOR SHELL         (I)  : 0.20900
REMARK 200  R SYM FOR SHELL           (I)  : 0.20900
REMARK 200  <I/SIGMA(I)> FOR SHELL          : 1.400
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT
REMARK 200 SOFTWARE USED: AMORE
REMARK 200 STARTING MODEL: PDB ENTRY 1EPF
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS    (%): NULL
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): NULL
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 14-17% PEG 4000, 450 MM LI SULFATE,
REMARK 280  100 MM NA ACETATE, PH 5.2, VAPOR DIFFUSION, HANGING DROP,
REMARK 280  TEMPERATURE 293K
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: I 21 21 21
REMARK 290
REMARK 290     SYMOP   SYMMETRY
REMARK 290     NNNMMM  OPERATOR
REMARK 290      1555   X,Y,Z
REMARK 290      2555   1/2-X,-Y,1/2+Z
REMARK 290      3555   -X,1/2+Y,1/2-Z
REMARK 290      4555   1/2+X,1/2-Y,-Z
REMARK 290      5555   1/2+X,1/2+Y,1/2+Z
REMARK 290      6555   -X,1/2-Y,Z
REMARK 290      7555   1/2-X,Y,-Z
REMARK 290      8555   X,-Y,1/2-Z
REMARK 290
REMARK 290     WHERE NNN -> OPERATOR NUMBER
REMARK 290           MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290     SMTRY1  1  1.000000  0.000000  0.000000        0.00000
REMARK 290     SMTRY2  1  0.000000  1.000000  0.000000        0.00000
REMARK 290     SMTRY3  1  0.000000  0.000000  1.000000        0.00000
REMARK 290     SMTRY1  2 -1.000000  0.000000  0.000000       25.72000
```

Figure 2 (Table 2 (page 5))

```
REMARK 290    SMTRY2   2  0.000000 -1.000000  0.000000         0.00000
REMARK 290    SMTRY3   2  0.000000  0.000000  1.000000        74.65000
REMARK 290    SMTRY1   3 -1.000000  0.000000  0.000000         0.00000
REMARK 290    SMTRY2   3  0.000000  1.000000  0.000000        53.88000
REMARK 290    SMTRY3   3  0.000000  0.000000 -1.000000        74.65000
REMARK 290    SMTRY1   4  1.000000  0.000000  0.000000        25.72000
REMARK 290    SMTRY2   4  0.000000 -1.000000  0.000000        53.88000
REMARK 290    SMTRY3   4  0.000000  0.000000 -1.000000         0.00000
REMARK 290    SMTRY1   5  1.000000  0.000000  0.000000        25.72000
REMARK 290    SMTRY2   5  0.000000  1.000000  0.000000        53.88000
REMARK 290    SMTRY3   5  0.000000  0.000000  1.000000        74.65000
REMARK 290    SMTRY1   6 -1.000000  0.000000  0.000000         0.00000
REMARK 290    SMTRY2   6  0.000000 -1.000000  0.000000        53.88000
REMARK 290    SMTRY3   6  0.000000  0.000000  1.000000         0.00000
REMARK 290    SMTRY1   7 -1.000000  0.000000  0.000000        25.72000
REMARK 290    SMTRY2   7  0.000000  1.000000  0.000000         0.00000
REMARK 290    SMTRY3   7  0.000000  0.000000 -1.000000         0.00000
REMARK 290    SMTRY1   8  1.000000  0.000000  0.000000         0.00000
REMARK 290    SMTRY2   8  0.000000 -1.000000  0.000000         0.00000
REMARK 290    SMTRY3   8  0.000000  0.000000 -1.000000        74.65000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
REMARK 300 WHICH CONSISTS OF 1 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 350
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW.  BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
REMARK 350    BIOMT1   1  1.000000  0.000000  0.000000         0.00000
REMARK 350    BIOMT2   1  0.000000  1.000000  0.000000         0.00000
REMARK 350    BIOMT3   1  0.000000  0.000000  1.000000         0.00000
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465   M RES C SSSEQI
REMARK 465     ARG A    -2
REMARK 465     GLU A   239
REMARK 465     GLU A   240
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
```

Figure 2 (Table 2(page 6))

```
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,3(1X,A4,2X),12X,F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500  M RES CSSEQI ATM1     ATM2     ATM3
REMARK 500    LEU A   1   N   -  CA   -  C    ANGL. DEV. = 11.0 DEGREES
REMARK 500    ASP A  27   N   -  CA   -  C    ANGL. DEV. = 11.4 DEGREES
REMARK 500    ALA A  28   N   -  CA   -  C    ANGL. DEV. =-17.5 DEGREES
REMARK 500    LYS A  29   N   -  CA   -  C    ANGL. DEV. = 12.7 DEGREES
REMARK 500    ASP A  56   N   -  CA   -  C    ANGL. DEV. =-11.4 DEGREES
REMARK 500    ALA A  89   N   -  CA   -  C    ANGL. DEV. =-10.5 DEGREES
REMARK 500    GLN A 108   N   -  CA   -  C    ANGL. DEV. =-10.5 DEGREES
REMARK 500    THR A 129   N   -  CA   -  C    ANGL. DEV. =-11.4 DEGREES
REMARK 500    ASP A 138   N   -  CA   -  C    ANGL. DEV. =-11.4 DEGREES
REMARK 500    ASP A 144   N   -  CA   -  C    ANGL. DEV. =-20.1 DEGREES
REMARK 500    THR A 194   N   -  CA   -  C    ANGL. DEV. =-11.0 DEGREES
REMARK 500    ARG A 257   N   -  CA   -  C    ANGL. DEV. = 17.3 DEGREES
REMARK 525
REMARK 525 SOLVENT
REMARK 525 THE FOLLOWING SOLVENT MOLECULES LIE FARTHER THAN EXPECTED
REMARK 525 FROM THE PROTEIN OR NUCLEIC ACID MOLECULE AND MAY BE
REMARK 525 ASSOCIATED WITH A SYMMETRY RELATED MOLECULE (M=MODEL
REMARK 525 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 525 NUMBER; I=INSERTION CODE):
REMARK 525
REMARK 525  M RES CSSEQI
REMARK 525    HOH    64        DISTANCE =  5.56 ANGSTROMS
REMARK 525    HOH    66        DISTANCE =  7.20 ANGSTROMS
REMARK 525    HOH    75        DISTANCE = 10.03 ANGSTROMS
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 2NCM    RELATED DB: PDB
REMARK 900 NMR STRUCTURE OF THE FIRST IMMUNOGLOBULIN DOMAIN OF THE
REMARK 900 NEURAL CELL ADHESION MOLECULE (NCAM)
REMARK 900 RELATED ID: 3NCM    RELATED DB: PDB
REMARK 900 NMR STRUCTURE OF THE SECOND IMMUNOGLOBULIN DOMAIN OF THE
REMARK 900 NEURAL CELL ADHESION MOLECULE (NCAM)
REMARK 900 RELATED ID: 1EPF    RELATED DB: PDB
REMARK 900 CRYSTAL STRUCTURE OF THE TWO N-TERMINAL IMMUNOGLOBULIN
REMARK 900 DOMAINS OF THE NEURAL CELL ADHESION MOLECULE (NCAM)
REMARK 999
REMARK 999 SEQUENCE
REMARK 999 RESIDUES -2, 239 AND 240 WERE NOT VISIBLE IN
REMARK 999 THE ELECTRON DENSITY.
DBREF  1QZ1 A    1   289  SWS    P13596    NCA1_RAT       20    308
SEQADV 1QZ1 ARG A   -2  SWS    P13596                CLONING ARTIFACT
SEQADV 1QZ1 VAL A   -1  SWS    P13596                CLONING ARTIFACT
SEQRES   1 A 291  ARG VAL LEU GLN VAL ASP ILE VAL PRO SER GLN GLY GLU
SEQRES   2 A 291  ILE SER VAL GLY GLU SER LYS PHE PHE LEU CYS GLN VAL
SEQRES   3 A 291  ALA GLY ASP ALA LYS ASP LYS ASP ILE SER TRP PHE SER
SEQRES   4 A 291  PRO ASN GLY GLU LYS LEU SER PRO ASN GLN GLN ARG ILE
SEQRES   5 A 291  SER VAL VAL TRP ASN ASP ASP SER SER THR LEU THR
SEQRES   6 A 291  ILE TYR ASN ALA ASN ILE ASP ASP ALA GLY ILE TYR LYS
SEQRES   7 A 291  CYS VAL VAL THR ALA GLU ASP GLY THR GLN SER GLU ALA
```

Figure 2 (Table 2 (page 7))

```
SEQRES   8  A 291    THR VAL ASN VAL LYS ILE PHE GLN LYS LEU MET PHE LYS
SEQRES   9  A 291    ASN ALA PRO THR PRO GLN GLU PHE LYS GLU GLY GLU ASP
SEQRES  10  A 291    ALA VAL ILE VAL CYS ASP VAL VAL SER SER LEU PRO PRO
SEQRES  11  A 291    THR ILE ILE TRP LYS HIS LYS GLY ARG ASP VAL ILE LEU
SEQRES  12  A 291    LYS LYS ASP VAL ARG PHE ILE VAL LEU SER ASN ASN TYR
SEQRES  13  A 291    LEU GLN ILE ARG GLY ILE LYS LYS THR ASP GLU GLY THR
SEQRES  14  A 291    TYR ARG CYS GLU GLY ARG ILE LEU ALA ARG GLY GLU ILE
SEQRES  15  A 291    ASN PHE LYS ASP ILE GLN VAL ILE VAL ASN VAL PRO PRO
SEQRES  16  A 291    THR VAL GLN ALA ARG GLN SER ILE VAL ASN ALA THR ALA
SEQRES  17  A 291    ASN LEU GLY GLN SER VAL THR LEU VAL CYS ASP ALA ASP
SEQRES  18  A 291    GLY PHE PRO GLU PRO THR MET SER TRP THR LYS ASP GLY
SEQRES  19  A 291    GLU PRO ILE GLU ASN GLU GLU GLU ASP ASP GLU LYS HIS
SEQRES  20  A 291    ILE PHE SER ASP ASP SER SER GLU LEU THR ILE ARG ASN
SEQRES  21  A 291    VAL ASP LYS ASN ASP GLU ALA GLU TYR VAL CYS ILE ALA
SEQRES  22  A 291    GLU ASN LYS ALA GLY GLU GLN ASP ALA SER ILE HIS LEU
SEQRES  23  A 291    LYS VAL PHE ALA LYS
FORMUL   2  HOH     *265(H2 O1)
HELIX    1   1 ASN A   68  ALA A   72  5                                    5
HELIX    2   2 LYS A  161  GLU A  165  5                                    5
HELIX    3   3 ASP A  260  GLU A  264  5                                    5
SHEET    1   A 4 VAL A    3  VAL A    6  0
SHEET    2   A 4 LYS A   18  VAL A   24 -1  O  GLN A   23   N  ASP A    4
SHEET    3   A 4 SER A   59  ILE A   64 -1  O  ILE A   64   N  LYS A   18
SHEET    4   A 4 ILE A   50  ASP A   56 -1  N  VAL A   53   O  THR A   61
SHEET    1   B 4 GLY A   10  SER A   13  0
SHEET    2   B 4 GLN A   86  PHE A   96  1  O  LYS A   94   N  GLY A    0
SHEET    3   B 4 GLY A   73  THR A   80 -1  N  VAL A   79   O  SER A   87
SHEET    4   B 4 ASP A   32  PHE A   36 -1  N  SER A   34   O  VAL A   78
SHEET    1   C 2 MET A  100  ASN A  103  0
SHEET    2   C 2 ASP A  121  VAL A  123 -1  O  ASP A  121   N  ASN A  103
SHEET    1   D 4 GLN A  108  LYS A  111  0
SHEET    2   D 4 GLU A  179  ALA A  197  1  O  ASN A  190   N  PHE A  110
SHEET    3   D 4 GLY A  166  ILE A  174 -1  N  GLY A  166   O  VAL A  187
SHEET    4   D 4 THR A  129  HIS A  134 -1  N  LYS A  133   O  ARG A  169
SHEET    1   E 5 GLN A  108  LYS A  111  0
SHEET    2   E 5 GLU A  179  ALA A  197  1  O  ASN A  190   N  PHE A  110
SHEET    3   E 5 VAL A  212  PHE A  221 -1  O  ASP A  217   N  GLN A  196
SHEET    4   E 5 GLU A  253  ILE A  256 -1  O  LEU A  254   N  LEU A  214
SHEET    5   E 5 HIS A  245  PHE A  247 -1  N  ILE A  246   O  THR A  255
SHEET    1   F 3 ALA A  116  ILE A  118  0
SHEET    2   F 3 LEU A  155  ILE A  157 -1  O  ILE A  157   N  ALA A  116
SHEET    3   F 3 PHE A  147  VAL A  149 -1  N  ILE A  148   O  GLN A  156
SHEET    1   G 5 ILE A  201  THR A  205  0
SHEET    2   G 5 GLY A  276  PHE A  287  1  O  PHE A  287   N  ALA A  204
SHEET    3   G 5 ALA A  265  ASN A  273 -1  N  TYR A  267   O  ILE A  282
SHEET    4   G 5 THR A  225  LYS A  230 -1  N  SER A  227   O  ILE A  270
SHEET    5   G 5 GLU A  233  PRO A  234 -1  O  GLU A  233   N  LYS A  230
SSBOND   1 CYS A   22    CYS A   77
SSBOND   2 CYS A  120    CYS A  170
SSBOND   3 CYS A  216    CYS A  269
CISPEP   1 VAL A    6    PRO A    7          0        -0.41
CISPEP   2 THR A  106    PRO A  107          0        -0.64
CISPEP   3 PHE A  221    PRO A  222          0        -0.72
CRYST1   51.440  107.760  149.300  90.00   90.00  90.00 I 21 21 21   8
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
```

Figure 2 (Table 2 (page 8))

```
SCALE1      0.019440  0.000000  0.000000      0.00000
SCALE2      0.000000  0.009280  0.000000      0.00000
SCALE3      0.000000  0.000000  0.006698      0.00000
ATOM     1   N   VAL A  -1     21.197  71.826 -24.060  1.00110.27  N
ATOM     2   CA  VAL A  -1     21.299  70.596 -24.891  1.00112.18  C
ATOM     3   C   VAL A  -1     20.583  69.411 -24.264  1.00111.88  C
ATOM     4   O   VAL A  -1     19.491  69.531 -23.699  1.00113.09  O
ATOM     5   CB  VAL A  -1     22.778  70.161 -25.114  1.00111.00  C
ATOM     6   CG1 VAL A  -1     23.591  71.324 -25.633  1.00109.72  C
ATOM     7   CG2 VAL A  -1     23.374  69.625 -23.817  1.00106.12  C
ATOM     8   N   LEU A   1     21.255  68.270 -24.364  1.00107.51  N
ATOM     9   CA  LEU A   1     20.778  66.981 -23.905  1.00100.28  C
ATOM    10   C   LEU A   1     20.360  66.739 -22.465  1.00 94.24  C
ATOM    11   O   LEU A   1     20.985  67.227 -21.518  1.00 93.77  O
ATOM    12   CB  LEU A   1     21.808  65.936 -24.296  1.00100.43  C
ATOM    13   CG  LEU A   1     21.297  64.909 -25.303  1.00103.11  C
ATOM    14   CD1 LEU A   1     20.253  65.528 -26.233  1.00106.65  C
ATOM    15   CD2 LEU A   1     22.475  64.366 -26.088  1.00101.88  C
ATOM    16   N   GLN A   2     19.299  65.946 -22.328  1.00 87.47  N
ATOM    17   CA  GLN A   2     18.771  65.575 -21.028  1.00 86.76  C
ATOM    18   C   GLN A   2     18.937  64.075 -20.822  1.00 80.18  C
ATOM    19   O   GLN A   2     18.520  63.264 -21.656  1.00 82.58  O
ATOM    20   CB  GLN A   2     17.292  65.950 -20.902  1.00 89.86  C
ATOM    21   CG  GLN A   2     16.819  65.996 -19.458  1.00102.22  C
ATOM    22   CD  GLN A   2     17.932  66.444 -18.500  1.00109.49  C
ATOM    23   OE1 GLN A   2     18.786  67.260 -18.859  1.00112.97  O
ATOM    24   NE2 GLN A   2     17.917  65.917 -17.275  1.00110.51  N
ATOM    25   N   VAL A   3     19.572  63.716 -19.714  1.00 68.44  N
ATOM    26   CA  VAL A   3     19.790  62.317 -19.375  1.00 65.80  C
ATOM    27   C   VAL A   3     19.290  62.058 -17.959  1.00 63.80  C
ATOM    28   O   VAL A   3     19.588  62.816 -17.029  1.00 61.99  O
ATOM    29   CB  VAL A   3     21.291  61.919 -19.495  1.00 70.09  C
ATOM    30   CG1 VAL A   3     22.157  62.831 -18.653  1.00 66.37  C
ATOM    31   CG2 VAL A   3     21.477  60.475 -19.072  1.00 53.43  C
ATOM    32   N   ASP A   4     18.511  60.992 -17.807  1.00 59.47  N
ATOM    33   CA  ASP A   4     17.957  60.635 -16.507  1.00 62.16  C
ATOM    34   C   ASP A   4     18.056  59.137 -16.281  1.00 61.45  C
ATOM    35   O   ASP A   4     17.973  58.337 -17.222  1.00 54.28  O
ATOM    36   CB  ASP A   4     16.490  61.064 -16.410  1.00 57.25  C
ATOM    37   CG  ASP A   4     16.312  62.564 -16.536  1.00 81.12  C
ATOM    38   OD1 ASP A   4     16.784  63.302 -15.644  1.00 87.44  O
ATOM    39   OD2 ASP A   4     15.702  63.010 -17.531  1.00 84.62  O
ATOM    40   N   ILE A   5     18.226  58.760 -15.024  1.00 54.90  N
ATOM    41   CA  ILE A   5     18.324  57.360 -14.692  1.00 47.24  C
ATOM    42   C   ILE A   5     17.134  56.965 -13.832  1.00 49.02  C
ATOM    43   O   ILE A   5     16.846  57.619 -12.826  1.00 47.37  O
ATOM    44   CB  ILE A   5     19.625  57.077 -13.934  1.00 42.30  C
ATOM    45   CG1 ILE A   5     20.823  57.333 -14.849  1.00 48.79  C
ATOM    46   CG2 ILE A   5     19.638  55.615 -13.450  1.00 40.90  C
ATOM    47   CD1 ILE A   5     22.158  57.356 -14.118  1.00 47.66  C
ATOM    48   N   VAL A   6     16.445  55.900 -14.233  1.00 48.39  N
ATOM    49   CA  VAL A   6     15.300  55.401 -13.480  1.00 48.78  C
ATOM    50   C   VAL A   6     15.545  53.939 -13.119  1.00 52.24  C
ATOM    51   O   VAL A   6     15.905  53.130 -13.980  1.00 51.37  O
ATOM    52   CB  VAL A   6     14.008  55.484 -14.299  1.00 55.65  C
ATOM    53   CG1 VAL A   6     12.857  54.882 -13.515  1.00 53.36  C
ATOM    54   CG2 VAL A   6     13.712  56.928 -14.637  1.00 64.21  C
```

Figure 2 (Table 2 (page 9))

ATOM	55	N	PRO	A	7	15.418	53.594	-11.830	1.00	44.55	N
ATOM	56	CA	PRO	A	7	15.074	54.460	-10.692	1.00	44.98	C
ATOM	57	C	PRO	A	7	16.225	55.428	-10.411	1.00	52.07	C
ATOM	58	O	PRO	A	7	17.391	55.112	-10.662	1.00	47.92	O
ATOM	59	CB	PRO	A	7	14.842	53.462	-9.556	1.00	50.48	C
ATOM	60	CG	PRO	A	7	15.718	52.291	-9.944	1.00	45.69	C
ATOM	61	CD	PRO	A	7	15.446	52.181	-11.420	1.00	40.86	C
ATOM	62	N	SER	A	8	15.894	56.604	-9.893	1.00	46.31	N
ATOM	63	CA	SER	A	8	16.889	57.635	-9.634	1.00	49.55	C
ATOM	64	C	SER	A	8	17.921	57.250	-8.592	1.00	53.48	C
ATOM	65	O	SER	A	8	18.995	57.857	-8.515	1.00	54.87	O
ATOM	66	CB	SER	A	8	16.198	58.940	-9.236	1.00	55.09	C
ATOM	67	OG	SER	A	8	15.363	58.753	-8.111	1.00	61.93	O
ATOM	68	N	GLN	A	9	17.597	56.255	-7.776	1.00	46.60	N
ATOM	69	CA	GLN	A	9	18.538	55.781	-6.771	1.00	47.40	C
ATOM	70	C	GLN	A	9	18.204	54.335	-6.448	1.00	44.46	C
ATOM	71	O	GLN	A	9	17.103	53.864	-6.739	1.00	52.34	O
ATOM	72	CB	GLN	A	9	18.494	56.658	-5.515	1.00	58.55	C
ATOM	73	CG	GLN	A	9	17.103	56.860	-4.900	1.00	65.92	C
ATOM	74	CD	GLN	A	9	17.149	57.765	-3.665	1.00	81.94	C
ATOM	75	OE1	GLN	A	9	17.878	57.484	-2.713	1.00	86.13	O
ATOM	76	NE2	GLN	A	9	16.374	58.853	-3.678	1.00	82.96	N
ATOM	77	N	GLY	A	10	19.157	53.606	-5.883	1.00	46.46	N
ATOM	78	CA	GLY	A	10	18.868	52.215	-5.589	1.00	50.99	C
ATOM	79	C	GLY	A	10	19.637	51.600	-4.442	1.00	48.97	C
ATOM	80	O	GLY	A	10	20.719	52.048	-4.070	1.00	46.47	O
ATOM	81	N	GLU	A	11	19.051	50.559	-3.871	1.00	54.04	N
ATOM	82	CA	GLU	A	11	19.684	49.842	-2.778	1.00	54.83	C
ATOM	83	C	GLU	A	11	19.560	48.362	-3.127	1.00	47.65	C
ATOM	84	O	GLU	A	11	18.499	47.918	-3.557	1.00	47.49	O
ATOM	85	CB	GLU	A	11	18.970	50.150	-1.456	1.00	49.30	C
ATOM	86	CG	GLU	A	11	19.627	49.508	-0.255	1.00	67.71	C
ATOM	87	CD	GLU	A	11	19.026	49.974	1.061	1.00	68.83	C
ATOM	88	OE1	GLU	A	11	17.829	49.704	1.305	1.00	70.78	O
ATOM	89	OE2	GLU	A	11	19.758	50.620	1.843	1.00	73.96	O
ATOM	90	N	ILE	A	12	20.636	47.599	-2.965	1.00	44.79	N
ATOM	91	CA	ILE	A	12	20.587	46.178	-3.302	1.00	43.25	C
ATOM	92	C	ILE	A	12	21.164	45.332	-2.185	1.00	49.76	C
ATOM	93	O	ILE	A	12	22.261	45.610	-1.692	1.00	45.49	O
ATOM	94	CB	ILE	A	12	21.402	45.856	-4.562	1.00	46.25	C
ATOM	95	CG1	ILE	A	12	21.182	46.938	-5.621	1.00	48.07	C
ATOM	96	CG2	ILE	A	12	20.984	44.481	-5.114	1.00	40.48	C
ATOM	97	CD1	ILE	A	12	22.125	46.814	-6.795	1.00	44.46	C
ATOM	98	N	SER	A	13	20.421	44.296	-1.796	1.00	50.25	N
ATOM	99	CA	SER	A	13	20.880	43.384	-0.755	1.00	49.85	C
ATOM	100	C	SER	A	13	21.869	42.416	-1.385	1.00	41.84	C
ATOM	101	O	SER	A	13	21.690	41.973	-2.526	1.00	43.99	O
ATOM	102	CB	SER	A	13	19.707	42.608	-0.156	1.00	48.85	C
ATOM	103	OG	SER	A	13	20.157	41.794	0.916	1.00	55.47	O
ATOM	104	N	VAL	A	14	22.926	42.114	-0.644	1.00	50.09	N
ATOM	105	CA	VAL	A	14	23.955	41.214	-1.126	1.00	48.58	C
ATOM	106	C	VAL	A	14	23.358	39.962	-1.742	1.00	53.11	C
ATOM	107	O	VAL	A	14	22.481	39.320	-1.165	1.00	54.25	O
ATOM	108	CB	VAL	A	14	24.924	40.814	0.004	1.00	51.58	C
ATOM	109	CG1	VAL	A	14	25.880	39.739	-0.479	1.00	51.54	C
ATOM	110	CG2	VAL	A	14	25.702	42.027	0.455	1.00	51.93	C
ATOM	111	N	GLY	A	15	23.841	39.636	-2.935	1.00	45.67	N

Figure 2 (Table 2 (page 10))

ATOM	112	CA	GLY	A	15	23.367	38.471	-3.643	1.00 45.80 C
ATOM	113	C	GLY	A	15	22.174	38.738	-4.546	1.00 49.51 C
ATOM	114	O	GLY	A	15	21.845	37.910	-5.395	1.00 44.42 O
ATOM	115	N	GLU	A	16	21.516	39.885	-4.390	1.00 48.69 N
ATOM	116	CA	GLU	A	16	20.360	40.167	-5.239	1.00 44.66 C
ATOM	117	C	GLU	A	16	20.712	41.010	-6.459	1.00 38.83 C
ATOM	118	O	GLU	A	16	21.874	41.355	-6.672	1.00 41.87 O
ATOM	119	CB	GLU	A	16	19.239	40.800	-4.403	1.00 44.40 C
ATOM	120	CG	GLU	A	16	18.799	39.848	-3.289	1.00 57.20 C
ATOM	121	CD	GLU	A	16	17.666	40.373	-2.428	1.00 67.70 C
ATOM	122	OE1	GLU	A	16	17.111	41.448	-2.739	1.00 72.10 O
ATOM	123	OE2	GLU	A	16	17.328	39.695	-1.433	1.00 77.10 O
ATOM	124	N	SER	A	17	19.712	41.319	-7.274	1.00 38.10 N
ATOM	125	CA	SER	A	17	19.950	42.068	-8.496	1.00 39.72 C
ATOM	126	C	SER	A	17	19.039	43.283	-8.655	1.00 43.71 C
ATOM	127	O	SER	A	17	17.960	43.330	-8.074	1.00 48.43 O
ATOM	128	CB	SER	A	17	19.787	41.125	-9.694	1.00 42.04 C
ATOM	129	OG	SER	A	17	20.672	40.016	-9.592	1.00 49.33 O
ATOM	130	N	LYS	A	18	19.491	44.273	-9.427	1.00 39.31 N
ATOM	131	CA	LYS	A	18	18.725	45.495	-9.689	1.00 40.44 C
ATOM	132	C	LYS	A	18	19.194	46.068	-11.004	1.00 36.17 C
ATOM	133	O	LYS	A	18	20.310	45.799	-11.447	1.00 41.18 O
ATOM	134	CB	LYS	A	18	18.944	46.552	-8.603	1.00 45.93 C
ATOM	135	CG	LYS	A	18	17.902	46.558	-7.506	1.00 63.96 C
ATOM	136	CD	LYS	A	18	17.343	47.954	-7.318	1.00 77.99 C
ATOM	137	CE	LYS	A	18	16.408	48.029	-6.120	1.00 91.67 C
ATOM	138	NZ	LYS	A	18	15.285	47.049	-6.198	1.00104.95 N
ATOM	139	N	PHE	A	19	18.355	46.866	-11.632	1.00 39.73 N
ATOM	140	CA	PHE	A	19	18.758	47.445	-12.889	1.00 42.56 C
ATOM	141	C	PHE	A	19	18.382	48.903	-12.907	1.00 45.52 C
ATOM	142	O	PHE	A	19	17.535	49.352	-12.123	1.00 41.88 O
ATOM	143	CB	PHE	A	19	18.131	46.681	-14.058	1.00 37.12 C
ATOM	144	CG	PHE	A	19	16.658	46.890	-14.220	1.00 41.51 C
ATOM	145	CD1	PHE	A	19	16.175	47.864	-15.090	1.00 45.13 C
ATOM	146	CD2	PHE	A	19	15.742	46.075	-13.547	1.00 42.50 C
ATOM	147	CE1	PHE	A	19	14.794	48.006	-15.310	1.00 44.84 C
ATOM	148	CE2	PHE	A	19	14.377	46.212	-13.759	1.00 43.30 C
ATOM	149	CZ	PHE	A	19	13.899	47.182	-14.639	1.00 41.52 C
ATOM	150	N	PHE	A	20	19.020	49.637	-13.813	1.00 37.54 N
ATOM	151	CA	PHE	A	20	18.816	51.062	-13.938	1.00 38.86 C
ATOM	152	C	PHE	A	20	18.816	51.437	-15.408	1.00 46.44 C
ATOM	153	O	PHE	A	20	19.702	51.035	-16.165	1.00 47.88 O
ATOM	154	CB	PHE	A	20	19.948	51.798	-13.205	1.00 36.96 C
ATOM	155	CG	PHE	A	20	20.112	51.368	-11.784	1.00 46.76 C
ATOM	156	CD1	PHE	A	20	20.904	50.267	-11.460	1.00 48.63 C
ATOM	157	CD2	PHE	A	20	19.427	52.027	-10.765	1.00 42.55 C
ATOM	158	CE1	PHE	A	20	21.008	49.826	-10.138	1.00 46.86 C
ATOM	159	CE2	PHE	A	20	19.525	51.591	-9.436	1.00 40.53 C
ATOM	160	CZ	PHE	A	20	20.317	50.489	-9.126	1.00 44.32 C
ATOM	161	N	LEU	A	21	17.816	52.209	-15.806	1.00 46.01 N
ATOM	162	CA	LEU	A	21	17.680	52.649	-17.189	1.00 49.63 C
ATOM	163	C	LEU	A	21	18.131	54.087	-17.360	1.00 46.97 C
ATOM	164	O	LEU	A	21	17.602	54.990	-16.719	1.00 43.22 O
ATOM	165	CB	LEU	A	21	16.218	52.530	-17.641	1.00 54.55 C
ATOM	166	CG	LEU	A	21	15.857	53.049	-19.040	1.00 57.21 C
ATOM	167	CD1	LEU	A	21	16.625	52.281	-20.096	1.00 58.14 C
ATOM	168	CD2	LEU	A	21	14.365	52.891	-19.274	1.00 55.27 C

Figure 2 (Table 2 (page 11))

ATOM	169	N	CYS A	22	19.122	54.291	-18.218	1.00	46.45	N
ATOM	170	CA	CYS A	22	19.615	55.628	-18.506	1.00	48.52	C
ATOM	171	C	CYS A	22	18.920	56.056	-19.788	1.00	54.42	C
ATOM	172	O	CYS A	22	19.157	55.478	-20.848	1.00	51.82	O
ATOM	173	CB	CYS A	22	21.115	55.601	-18.730	1.00	49.72	C
ATOM	174	SG	CYS A	22	21.827	57.215	-19.167	1.00	55.16	S
ATOM	175	N	GLN A	23	18.069	57.071	-19.689	1.00	59.11	N
ATOM	176	CA	GLN A	23	17.312	57.546	-20.837	1.00	66.68	C
ATOM	177	C	GLN A	23	17.718	58.941	-21.314	1.00	63.21	C
ATOM	178	O	GLN A	23	17.951	59.839	-20.509	1.00	57.50	O
ATOM	179	CB	GLN A	23	15.825	57.547	-20.482	1.00	69.27	C
ATOM	180	CG	GLN A	23	14.900	57.940	-21.618	1.00	83.38	C
ATOM	181	CD	GLN A	23	14.575	56.779	-22.549	1.00	90.68	C
ATOM	182	OE1	GLN A	23	14.251	55.685	-22.089	1.00	97.59	O
ATOM	183	NE2	GLN A	23	14.642	57.016	-23.861	1.00	95.34	N
ATOM	184	N	VAL A	24	17.799	59.118	-22.629	1.00	67.26	N
ATOM	185	CA	VAL A	24	18.145	60.415	-23.197	1.00	74.82	C
ATOM	186	C	VAL A	24	16.857	61.028	-23.739	1.00	75.90	C
ATOM	187	O	VAL A	24	16.039	60.338	-24.356	1.00	76.41	O
ATOM	188	CB	VAL A	24	19.178	60.285	-24.343	1.00	77.43	C
ATOM	189	CG1	VAL A	24	19.560	61.657	-24.852	1.00	77.38	C
ATOM	190	CG2	VAL A	24	20.418	59.547	-23.856	1.00	81.07	C
ATOM	191	N	ALA A	25	16.685	62.324	-23.500	1.00	82.73	N
ATOM	192	CA	ALA A	25	15.490	63.053	-23.933	1.00	92.22	C
ATOM	193	C	ALA A	25	15.455	63.428	-25.424	1.00	99.21	C
ATOM	194	O	ALA A	25	16.491	63.734	-26.019	1.00	99.63	O
ATOM	195	CB	ALA A	25	15.326	64.307	-23.078	1.00	89.44	C
ATOM	196	N	GLY A	26	14.249	63.405	-26.002	1.00107.66	N
ATOM	197	CA	GLY A	26	14.040	63.735	-27.410	1.00117.13	C
ATOM	198	C	GLY A	26	14.697	62.739	-28.348	1.00123.74	C
ATOM	199	O	GLY A	26	14.060	62.088	-29.188	1.00126.85	O
ATOM	200	N	ASP A	27	16.010	62.671	-28.187	1.00127.93	N
ATOM	201	CA	ASP A	27	16.915	61.795	-28.897	1.00131.73	C
ATOM	202	C	ASP A	27	17.049	61.809	-30.410	1.00132.38	C
ATOM	203	O	ASP A	27	16.518	60.944	-31.112	1.00134.43	O
ATOM	204	CB	ASP A	27	16.721	60.353	-28.433	1.00133.67	C
ATOM	205	CG	ASP A	27	17.976	59.540	-28.620	1.00136.05	C
ATOM	206	OD1	ASP A	27	19.011	60.177	-28.888	1.00137.46	O
ATOM	207	OD2	ASP A	27	17.940	58.305	-28.501	1.00138.22	O
ATOM	208	N	ALA A	28	17.776	62.812	-30.894	1.00130.01	N
ATOM	209	CA	ALA A	28	18.098	62.888	-32.301	1.00127.19	C
ATOM	210	C	ALA A	28	19.203	61.826	-32.208	1.00125.97	C
ATOM	211	O	ALA A	28	19.562	61.453	-31.091	1.00125.76	O
ATOM	212	CB	ALA A	28	18.672	64.248	-32.657	1.00123.21	C
ATOM	213	N	LYS A	29	19.777	61.332	-33.300	1.00124.23	N
ATOM	214	CA	LYS A	29	20.754	60.267	-33.095	1.00120.04	C
ATOM	215	C	LYS A	29	22.237	60.419	-33.356	1.00114.93	C
ATOM	216	O	LYS A	29	22.773	61.503	-33.593	1.00109.02	O
ATOM	217	CB	LYS A	29	20.254	58.988	-33.777	1.00124.97	C
ATOM	218	CG	LYS A	29	19.095	58.340	-33.030	1.00125.66	C
ATOM	219	CD	LYS A	29	18.639	57.047	-33.674	1.00125.32	C
ATOM	220	CE	LYS A	29	17.462	56.460	-32.915	1.00120.15	C
ATOM	221	NZ	LYS A	29	16.388	57.477	-32.740	1.00120.03	N
ATOM	222	N	ASP A	30	22.875	59.260	-33.286	1.00110.94	N
ATOM	223	CA	ASP A	30	24.297	59.108	-33.440	1.00108.72	C
ATOM	224	C	ASP A	30	25.004	59.738	-32.257	1.00102.56	C
ATOM	225	O	ASP A	30	25.869	60.592	-32.425	1.00101.55	O

Figure 2 (Table 2 (page 12))

```
ATOM    226  CB   ASP A  30      24.800  59.729 -34.740  1.00114.65  C
ATOM    227  CG   ASP A  30      25.573  58.735 -35.584  1.00121.84  C
ATOM    228  OD1  ASP A  30      26.219  57.833 -35.001  1.00126.50  O
ATOM    229  OD2  ASP A  30      25.543  58.853 -36.824  1.00125.16  O
ATOM    230  N    LYS A  31      24.602  59.339 -31.055  1.00 90.62  N
ATOM    231  CA   LYS A  31      25.252  59.820 -29.845  1.00 86.82  C
ATOM    232  C    LYS A  31      25.645  58.547 -29.120  1.00 76.37  C
ATOM    233  O    LYS A  31      25.000  57.512 -29.280  1.00 76.59  O
ATOM    234  CB   LYS A  31      24.315  60.658 -28.965  1.00 87.55  C
ATOM    235  CG   LYS A  31      23.238  59.873 -28.261  1.00 90.62  C
ATOM    236  CD   LYS A  31      21.906  60.210 -28.856  1.00 90.82  C
ATOM    237  CE   LYS A  31      21.081  58.968 -28.999  1.00 94.15  C
ATOM    238  NZ   LYS A  31      20.424  58.901 -30.339  1.00 96.17  N
ATOM    239  N    ASP A  32      26.711  58.620 -28.341  1.00 66.33  N
ATOM    240  CA   ASP A  32      27.202  57.467 -27.607  1.00 64.69  C
ATOM    241  C    ASP A  32      26.732  57.503 -26.163  1.00 57.45  C
ATOM    242  O    ASP A  32      26.707  58.563 -25.532  1.00 61.27  O
ATOM    243  CB   ASP A  32      28.740  57.448 -27.669  1.00 59.49  C
ATOM    244  CG   ASP A  32      29.372  56.362 -26.791  1.00 67.93  C
ATOM    245  OD1  ASP A  32      29.627  56.626 -25.589  1.00 51.53  O
ATOM    246  OD2  ASP A  32      29.626  55.248 -27.308  1.00 61.79  O
ATOM    247  N    ILE A  33      26.336  56.342 -25.657  1.00 54.91  N
ATOM    248  CA   ILE A  33      25.911  56.210 -24.271  1.00 52.46  C
ATOM    249  C    ILE A  33      26.823  55.173 -23.640  1.00 53.58  C
ATOM    250  O    ILE A  33      26.875  54.022 -24.083  1.00 50.96  O
ATOM    251  CB   ILE A  33      24.470  55.712 -24.139  1.00 51.31  C
ATOM    252  CG1  ILE A  33      23.518  56.700 -24.800  1.00 52.96  C
ATOM    253  CG2  ILE A  33      24.116  55.563 -22.654  1.00 50.09  C
ATOM    254  CD1  ILE A  33      22.087  56.233 -24.828  1.00 54.31  C
ATOM    255  N    SER A  34      27.535  55.588 -22.603  1.00 43.80  N
ATOM    256  CA   SER A  34      28.463  54.716 -21.910  1.00 47.69  C
ATOM    257  C    SER A  34      28.262  54.831 -20.410  1.00 51.46  C
ATOM    258  O    SER A  34      27.899  55.892 -19.897  1.00 50.26  O
ATOM    259  CB   SER A  34      29.898  55.105 -22.255  1.00 44.86  C
ATOM    260  OG   SER A  34      30.197  54.768 -23.592  1.00 56.99  O
ATOM    261  N    TRP A  35      28.488  53.726 -19.714  1.00 47.72  N
ATOM    262  CA   TRP A  35      28.359  53.713 -18.270  1.00 42.75  C
ATOM    263  C    TRP A  35      29.741  53.598 -17.652  1.00 45.12  C
ATOM    264  O    TRP A  35      30.640  52.967 -18.223  1.00 44.07  O
ATOM    265  CB   TRP A  35      27.511  52.531 -17.800  1.00 39.02  C
ATOM    266  CG   TRP A  35      26.028  52.667 -18.015  1.00 43.96  C
ATOM    267  CD1  TRP A  35      25.323  52.308 -19.126  1.00 38.82  C
ATOM    268  CD2  TRP A  35      25.062  53.080 -17.041  1.00 36.18  C
ATOM    269  NE1  TRP A  35      23.974  52.454 -18.901  1.00 45.99  N
ATOM    270  CE2  TRP A  35      23.786  52.925 -17.632  1.00 47.03  C
ATOM    271  CE3  TRP A  35      25.150  53.556 -15.735  1.00 39.81  C
ATOM    272  CZ2  TRP A  35      22.605  53.232 -16.948  1.00 43.25  C
ATOM    273  CZ3  TRP A  35      23.962  53.865 -15.054  1.00 41.38  C
ATOM    274  CH2  TRP A  35      22.713  53.699 -15.668  1.00 42.80  C
ATOM    275  N    PHE A  36      29.907  54.225 -16.491  1.00 45.19  N
ATOM    276  CA   PHE A  36      31.160  54.178 -15.748  1.00 44.89  C
ATOM    277  C    PHE A  36      30.834  53.716 -14.345  1.00 44.82  C
ATOM    278  O    PHE A  36      29.858  54.166 -13.755  1.00 41.52  O
ATOM    279  CB   PHE A  36      31.819  55.556 -15.675  1.00 43.10  C
ATOM    280  CG   PHE A  36      32.286  56.062 -17.006  1.00 55.53  C
ATOM    281  CD1  PHE A  36      31.385  56.639 -17.893  1.00 51.14  C
ATOM    282  CD2  PHE A  36      33.610  55.883 -17.407  1.00 46.89  C
```

Figure 2 (Table 2 (page 13))

ATOM	283	CE1	PHE	A	36	31.789	57.030	-19.173	1.00	54.91	C
ATOM	284	CE2	PHE	A	36	34.030	56.269	-18.684	1.00	55.64	C
ATOM	285	CZ	PHE	A	36	33.110	56.846	-19.573	1.00	50.29	C
ATOM	286	N	SER	A	37	31.641	52.795	-13.832	1.00	42.90	N
ATOM	287	CA	SER	A	37	31.447	52.289	-12.488	1.00	52.59	C
ATOM	288	C	SER	A	37	31.973	53.321	-11.490	1.00	53.66	C
ATOM	289	O	SER	A	37	32.581	54.325	-11.878	1.00	46.56	O
ATOM	290	CB	SER	A	37	32.176	50.950	-12.322	1.00	56.49	C
ATOM	291	OG	SER	A	37	33.540	51.055	-12.675	1.00	54.60	O
ATOM	292	N	PRO	A	38	31.729	53.096	-10.192	1.00	55.82	N
ATOM	293	CA	PRO	A	38	32.169	54.004	-9.124	1.00	58.18	C
ATOM	294	C	PRO	A	38	33.682	54.241	-9.057	1.00	56.07	C
ATOM	295	O	PRO	A	38	34.135	55.248	-8.519	1.00	57.12	O
ATOM	296	CB	PRO	A	38	31.619	53.338	-7.864	1.00	55.81	C
ATOM	297	CG	PRO	A	38	30.327	52.731	-8.377	1.00	51.53	C
ATOM	298	CD	PRO	A	38	30.764	52.107	-9.677	1.00	50.32	C
ATOM	299	N	ASN	A	39	34.456	53.317	-9.609	1.00	52.69	N
ATOM	300	CA	ASN	A	39	35.905	53.452	-9.613	1.00	59.02	C
ATOM	301	C	ASN	A	39	36.396	54.175	-10.881	1.00	61.73	C
ATOM	302	O	ASN	A	39	37.585	54.160	-11.188	1.00	57.13	O
ATOM	303	CB	ASN	A	39	36.551	52.077	-9.523	1.00	56.75	C
ATOM	304	CG	ASN	A	39	36.432	51.310	-10.810	1.00	71.38	C
ATOM	305	OD1	ASN	A	39	35.531	51.565	-11.603	1.00	73.88	O
ATOM	306	ND2	ASN	A	39	37.332	50.361	-11.027	1.00	79.44	N
ATOM	307	N	GLY	A	40	35.471	54.777	-11.626	1.00	54.18	N
ATOM	308	CA	GLY	A	40	35.839	55.523	-12.825	1.00	58.26	C
ATOM	309	C	GLY	A	40	36.049	54.777	-14.126	1.00	56.72	C
ATOM	310	O	GLY	A	40	36.311	55.385	-15.161	1.00	59.14	O
ATOM	311	N	GLU	A	41	35.940	53.462	-14.098	1.00	53.24	N
ATOM	312	CA	GLU	A	41	36.137	52.712	-15.312	1.00	54.15	C
ATOM	313	C	GLU	A	41	34.887	52.572	-16.152	1.00	52.64	C
ATOM	314	O	GLU	A	41	33.772	52.444	-15.645	1.00	51.92	O
ATOM	315	CB	GLU	A	41	36.695	51.341	-14.988	1.00	62.00	C
ATOM	316	CG	GLU	A	41	38.100	51.410	-14.451	1.00	86.56	C
ATOM	317	CD	GLU	A	41	38.565	50.074	-13.931	1.00	94.84	C
ATOM	318	OE1	GLU	A	41	37.901	49.059	-14.243	1.00	99.92	O
ATOM	319	OE2	GLU	A	41	39.591	50.041	-13.220	1.00	98.17	O
ATOM	320	N	LYS	A	42	35.104	52.625	-17.457	1.00	48.52	N
ATOM	321	CA	LYS	A	42	34.050	52.475	-18.430	1.00	45.24	C
ATOM	322	C	LYS	A	42	33.714	50.979	-18.477	1.00	52.84	C
ATOM	323	O	LYS	A	42	34.607	50.126	-18.534	1.00	47.42	O
ATOM	324	CB	LYS	A	42	34.536	52.971	-19.796	1.00	46.19	C
ATOM	325	CG	LYS	A	42	33.502	52.863	-20.930	1.00	58.73	C
ATOM	326	CD	LYS	A	42	34.006	53.553	-22.205	1.00	60.30	C
ATOM	327	CE	LYS	A	42	33.004	53.446	-23.353	1.00	69.24	C
ATOM	328	NZ	LYS	A	42	33.486	54.104	-24.606	1.00	73.95	N
ATOM	329	N	LEU	A	43	32.425	50.659	-18.441	1.00	42.58	N
ATOM	330	CA	LEU	A	43	31.986	49.270	-18.453	1.00	44.33	C
ATOM	331	C	LEU	A	43	31.907	48.724	-19.863	1.00	45.36	C
ATOM	332	O	LEU	A	43	31.315	49.351	-20.734	1.00	49.42	O
ATOM	333	CB	LEU	A	43	30.613	49.177	-17.778	1.00	37.59	C
ATOM	334	CG	LEU	A	43	30.672	49.579	-16.302	1.00	45.02	C
ATOM	335	CD1	LEU	A	43	29.276	49.708	-15.713	1.00	48.59	C
ATOM	336	CD2	LEU	A	43	31.489	48.538	-15.550	1.00	45.09	C
ATOM	337	N	SER	A	44	32.507	47.566	-20.100	0.50	34.43	N
ATOM	338	CA	SER	A	44	32.436	46.990	-21.429	0.50	37.54	C
ATOM	339	C	SER	A	44	31.017	46.509	-21.595	0.50	40.70	C

Figure 2 (Table 2 (page 14))

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ATOM    340   O    SER A   44      30.404   45.984  -20.672   0.50  31.07  O
ATOM    341   CB   SER A   44      33.394   45.813  -21.590   0.50  34.76  C
ATOM    342   OG   SER A   44      34.730   46.238  -21.418   0.50  37.63  O
ATOM    343   N    PRO A   45      30.475   46.684  -22.787   1.00  55.79  N
ATOM    344   CA   PRO A   45      29.104   46.261  -23.062   1.00  56.53  C
ATOM    345   C    PRO A   45      28.910   44.761  -23.041   1.00  53.37  C
ATOM    346   O    PRO A   45      29.849   43.986  -23.229   1.00  56.21  O
ATOM    347   CB   PRO A   45      28.836   46.833  -24.458   1.00  60.37  C
ATOM    348   CG   PRO A   45      29.823   47.960  -24.586   1.00  60.02  C
ATOM    349   CD   PRO A   45      31.056   47.392  -23.941   1.00  63.21  C
ATOM    350   N    ASN A   46      27.667   44.370  -22.800   1.00  57.48  N
ATOM    351   CA   ASN A   46      27.279   42.973  -22.812   1.00  57.72  C
ATOM    352   C    ASN A   46      28.150   41.993  -22.017   1.00  57.75  C
ATOM    353   O    ASN A   46      28.534   40.950  -22.541   1.00  60.65  O
ATOM    354   CB   ASN A   46      27.179   42.508  -24.272   1.00  67.80  C
ATOM    355   CG   ASN A   46      26.285   43.417  -25.119   1.00  71.96  C
ATOM    356   OD1  ASN A   46      25.090   43.557  -24.850   1.00  81.33  O
ATOM    357   ND2  ASN A   46      26.862   44.033  -26.146   1.00  70.84  N
ATOM    358   N    GLN A   47      28.478   42.325  -20.771   1.00  53.34  N
ATOM    359   CA   GLN A   47      29.250   41.408  -19.925   1.00  49.41  C
ATOM    360   C    GLN A   47      28.202   40.672  -19.091   1.00  50.32  C
ATOM    361   O    GLN A   47      27.029   41.040  -19.111   1.00  47.47  O
ATOM    362   CB   GLN A   47      30.232   42.156  -19.022   1.00  51.46  C
ATOM    363   CG   GLN A   47      31.291   42.936  -19.798   1.00  49.02  C
ATOM    364   CD   GLN A   47      32.023   42.055  -20.812   1.00  60.54  C
ATOM    365   OE1  GLN A   47      32.910   41.286  -20.448   1.00  52.30  O
ATOM    366   NE2  GLN A   47      31.634   42.149  -22.082   1.00  51.19  N
ATOM    367   N    GLN A   48      28.630   39.669  -18.336   1.00  52.29  N
ATOM    368   CA   GLN A   48      27.728   38.807  -17.566   1.00  56.49  C
ATOM    369   C    GLN A   48      27.049   39.337  -16.305   1.00  58.23  C
ATOM    370   O    GLN A   48      25.818   39.453  -16.238   1.00  50.89  O
ATOM    371   CB   GLN A   48      28.486   37.524  -17.199   1.00  69.79  C
ATOM    372   CG   GLN A   48      27.606   36.324  -16.903   1.00  85.42  C
ATOM    373   CD   GLN A   48      27.071   35.675  -18.172   1.00  96.52  C
ATOM    374   OE1  GLN A   48      27.848   35.302  -19.052   1.00 103.65  O
ATOM    375   NE2  GLN A   48      25.745   35.530  -18.272   1.00  97.26  N
ATOM    376   N    ARG A   49      27.866   39.613  -15.297   1.00  46.27  N
ATOM    377   CA   ARG A   49      27.376   40.069  -14.009   1.00  49.02  C
ATOM    378   C    ARG A   49      27.031   41.558  -13.965   1.00  50.34  C
ATOM    379   O    ARG A   49      25.951   41.929  -13.518   1.00  44.46  O
ATOM    380   CB   ARG A   49      28.404   39.724  -12.937   1.00  43.05  C
ATOM    381   CG   ARG A   49      27.841   39.691  -11.541   1.00  50.00  C
ATOM    382   CD   ARG A   49      28.920   39.301  -10.560   1.00  46.14  C
ATOM    383   NE   ARG A   49      29.847   40.402  -10.332   1.00  50.29  N
ATOM    384   CZ   ARG A   49      29.552   41.479   -9.614   1.00  49.75  C
ATOM    385   NH1  ARG A   49      28.355   41.602   -9.054   1.00  46.61  N
ATOM    386   NH2  ARG A   49      30.456   42.434   -9.450   1.00  54.16  N
ATOM    387   N    ILE A   50      27.950   42.413  -14.404   1.00  45.13  N
ATOM    388   CA   ILE A   50      27.693   43.846  -14.431   1.00  47.45  C
ATOM    389   C    ILE A   50      27.362   44.081  -15.886   1.00  49.10  C
ATOM    390   O    ILE A   50      28.236   44.288  -16.718   1.00  46.05  O
ATOM    391   CB   ILE A   50      28.927   44.633  -13.989   1.00  46.67  C
ATOM    392   CG1  ILE A   50      29.309   44.197  -12.569   1.00  49.39  C
ATOM    393   CG2  ILE A   50      28.645   46.122  -14.047   1.00  45.96  C
ATOM    394   CD1  ILE A   50      28.175   44.305  -11.547   1.00  38.44  C
ATOM    395   N    SER A   51      26.069   44.019  -16.172   1.00  45.97  N
ATOM    396   CA   SER A   51      25.572   44.111  -17.523   1.00  42.85  C
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Figure 2 (Table 2 (page 15))

ATOM	397	C	SER	A	51	25.123	45.464	-18.027	1.00 47.59	C
ATOM	398	O	SER	A	51	24.300	46.145	-17.408	1.00 47.20	O
ATOM	399	CB	SER	A	51	24.430	43.096	-17.676	1.00 42.67	C
ATOM	400	OG	SER	A	51	23.643	43.375	-18.811	1.00 55.89	O
ATOM	401	N	VAL	A	52	25.689	45.856	-19.159	1.00 45.49	N
ATOM	402	CA	VAL	A	52	25.317	47.100	-19.802	1.00 46.68	C
ATOM	403	C	VAL	A	52	24.768	46.706	-21.155	1.00 52.16	C
ATOM	404	O	VAL	A	52	25.483	46.140	-21.991	1.00 52.43	O
ATOM	405	CB	VAL	A	52	26.504	48.038	-20.028	1.00 51.87	C
ATOM	406	CG1	VAL	A	52	26.064	49.202	-20.901	1.00 49.68	C
ATOM	407	CG2	VAL	A	52	27.029	48.555	-18.694	1.00 46.22	C
ATOM	408	N	VAL	A	53	23.491	46.999	-21.353	1.00 43.80	N
ATOM	409	CA	VAL	A	53	22.813	46.679	-22.584	1.00 51.71	C
ATOM	410	C	VAL	A	53	22.126	47.901	-23.192	1.00 60.49	C
ATOM	411	O	VAL	A	53	21.288	48.550	-22.564	1.00 55.82	O
ATOM	412	CB	VAL	A	53	21.770	45.573	-22.343	1.00 57.05	C
ATOM	413	CG1	VAL	A	53	20.897	45.392	-23.569	1.00 61.58	C
ATOM	414	CG2	VAL	A	53	22.478	44.269	-22.008	1.00 51.45	C
ATOM	415	N	TRP	A	54	22.511	48.205	-24.422	1.00 65.48	N
ATOM	416	CA	TRP	A	54	21.948	49.309	-25.178	1.00 74.11	C
ATOM	417	C	TRP	A	54	20.581	48.813	-25.650	1.00 74.48	C
ATOM	418	O	TRP	A	54	20.475	47.706	-26.167	1.00 72.95	O
ATOM	419	CB	TRP	A	54	22.851	49.571	-26.365	1.00 82.17	C
ATOM	420	CG	TRP	A	54	22.565	50.791	-27.135	1.00 99.79	C
ATOM	421	CD1	TRP	A	54	22.877	52.073	-26.787	1.00102.50	C
ATOM	422	CD2	TRP	A	54	22.021	50.849	-28.456	1.00107.53	C
ATOM	423	NE1	TRP	A	54	22.573	52.929	-27.817	1.00109.34	N
ATOM	424	CE2	TRP	A	54	22.045	52.205	-28.852	1.00111.35	C
ATOM	425	CE3	TRP	A	54	21.515	49.889	-29.343	1.00108.73	C
ATOM	426	CZ2	TRP	A	54	21.590	52.619	-30.108	1.00112.86	C
ATOM	427	CZ3	TRP	A	54	21.061	50.305	-30.591	1.00109.55	C
ATOM	428	CH2	TRP	A	54	21.100	51.662	-30.959	1.00110.38	C
ATOM	429	N	ASN	A	55	19.537	49.612	-25.471	1.00 71.63	N
ATOM	430	CA	ASN	A	55	18.205	49.185	-25.878	1.00 76.76	C
ATOM	431	C	ASN	A	55	17.845	49.651	-27.281	1.00 81.91	C
ATOM	432	O	ASN	A	55	17.573	48.846	-28.168	1.00 88.33	O
ATOM	433	CB	ASN	A	55	17.197	49.689	-24.858	1.00 71.55	C
ATOM	434	CG	ASN	A	55	17.474	49.141	-23.476	1.00 75.04	C
ATOM	435	OD1	ASN	A	55	17.374	47.932	-23.246	1.00 72.25	O
ATOM	436	ND2	ASN	A	55	17.841	50.021	-22.550	1.00 50.95	N
ATOM	437	N	ASP	A	56	17.833	50.962	-27.455	1.00 88.42	N
ATOM	438	CA	ASP	A	56	17.548	51.607	-28.722	1.00 96.25	C
ATOM	439	C	ASP	A	56	18.566	52.727	-28.677	1.00101.81	C
ATOM	440	O	ASP	A	56	19.369	52.797	-27.736	1.00102.77	O
ATOM	441	CB	ASP	A	56	16.107	52.147	-28.744	1.00 95.48	C
ATOM	442	CG	ASP	A	56	15.707	52.811	-27.433	1.00 93.76	C
ATOM	443	OD1	ASP	A	56	16.451	53.704	-26.985	1.00 85.05	O
ATOM	444	OD2	ASP	A	56	14.658	52.452	-26.849	1.00 93.98	O
ATOM	445	N	ASP	A	57	18.599	53.607	-29.663	1.00102.50	N
ATOM	446	CA	ASP	A	57	19.610	54.674	-29.562	1.00102.11	C
ATOM	447	C	ASP	A	57	19.218	55.678	-28.491	1.00 97.41	C
ATOM	448	O	ASP	A	57	19.933	56.652	-28.258	1.00 97.40	O
ATOM	449	CB	ASP	A	57	19.781	55.395	-30.900	1.00112.19	C
ATOM	450	CG	ASP	A	57	21.068	56.116	-30.995	1.00121.70	C
ATOM	451	OD1	ASP	A	57	21.660	56.543	-29.959	1.00128.34	O
ATOM	452	OD2	ASP	A	57	21.589	56.364	-32.125	1.00123.94	O
ATOM	453	N	ASP	A	58	18.084	55.433	-27.843	1.00 90.49	N

Figure 2 (Table 2 (page 16))

```
ATOM    454  CA   ASP A   58      17.622  56.352  -26.826   1.00  87.06   C
ATOM    455  C    ASP A   58      18.071  55.997  -25.427   1.00  73.82   C
ATOM    456  O    ASP A   58      18.180  56.880  -24.577   1.00  62.84   O
ATOM    457  CB   ASP A   58      16.093  56.433  -26.809   1.00103.58   C
ATOM    458  CG   ASP A   58      15.487  56.564  -28.191   1.00113.84   C
ATOM    459  OD1  ASP A   58      15.498  57.677  -28.763   1.00117.69   O
ATOM    460  OD2  ASP A   58      14.997  55.534  -28.700   1.00121.72   O
ATOM    461  N    SER A   59      18.320  54.717  -25.174   1.00  64.75   N
ATOM    462  CA   SER A   59      18.681  54.313  -23.828   1.00  61.90   C
ATOM    463  C    SER A   59      19.628  53.131  -23.689   1.00  64.15   C
ATOM    464  O    SER A   59      19.869  52.359  -24.627   1.00  60.43   O
ATOM    465  CB   SER A   59      17.408  54.000  -23.052   1.00  55.02   C
ATOM    466  OG   SER A   59      16.760  52.881  -23.625   1.00  62.54   O
ATOM    467  N    SER A   60      20.145  53.005  -22.473   1.00  58.32   N
ATOM    468  CA   SER A   60      21.062  51.941  -22.111   1.00  53.12   C
ATOM    469  C    SER A   60      20.694  51.465  -20.708   1.00  51.38   C
ATOM    470  O    SER A   60      20.439  52.271  -19.815   1.00  50.11   O
ATOM    471  CB   SER A   60      22.502  52.451  -22.127   1.00  48.06   C
ATOM    472  OG   SER A   60      23.407  51.420  -21.751   1.00  54.93   O
ATOM    473  N    THR A   61      20.667  50.157  -20.509   1.00  41.41   N
ATOM    474  CA   THR A   61      20.308  49.618  -19.206   1.00  44.19   C
ATOM    475  C    THR A   61      21.489  48.979  -18.501   1.00  42.41   C
ATOM    476  O    THR A   61      22.227  48.188  -19.081   1.00  46.93   O
ATOM    477  CB   THR A   61      19.183  48.583  -19.353   1.00  47.49   C
ATOM    478  OG1  THR A   61      18.023  49.233  -19.880   1.00  56.06   O
ATOM    479  CG2  THR A   61      18.837  47.945  -18.004   1.00  45.18   C
ATOM    480  N    LEU A   62      21.674  49.359  -17.247   1.00  37.61   N
ATOM    481  CA   LEU A   62      22.731  48.797  -16.432   1.00  39.04   C
ATOM    482  C    LEU A   62      22.076  47.810  -15.475   1.00  38.19   C
ATOM    483  O    LEU A   62      21.171  48.185  -14.722   1.00  38.43   O
ATOM    484  CB   LEU A   62      23.431  49.896  -15.628   1.00  34.82   C
ATOM    485  CG   LEU A   62      24.273  49.373  -14.461   1.00  46.86   C
ATOM    486  CD1  LEU A   62      25.418  48.550  -14.996   1.00  41.11   C
ATOM    487  CD2  LEU A   62      24.797  50.517  -13.617   1.00  40.98   C
ATOM    488  N    THR A   63      22.488  46.548  -15.514   1.00  34.32   N
ATOM    489  CA   THR A   63      21.930  45.570  -14.583   1.00  42.11   C
ATOM    490  C    THR A   63      23.043  45.058  -13.694   1.00  38.02   C
ATOM    491  O    THR A   63      24.086  44.634  -14.181   1.00  39.91   O
ATOM    492  CB   THR A   63      21.312  44.333  -15.284   1.00  44.60   C
ATOM    493  OG1  THR A   63      20.291  44.746  -16.193   1.00  38.13   O
ATOM    494  CG2  THR A   63      20.709  43.388  -14.247   1.00  41.53   C
ATOM    495  N    ILE A   64      22.831  45.096  -12.390   1.00  32.30   N
ATOM    496  CA   ILE A   64      23.835  44.596  -11.464   1.00  40.27   C
ATOM    497  C    ILE A   64      23.288  43.299  -10.884   1.00  44.61   C
ATOM    498  O    ILE A   64      22.400  43.324  -10.032   1.00  43.38   O
ATOM    499  CB   ILE A   64      24.116  45.600  -10.319   1.00  43.07   C
ATOM    500  CG1  ILE A   64      24.757  46.868  -10.894   1.00  50.00   C
ATOM    501  CG2  ILE A   64      25.032  44.962   -9.265   1.00  36.35   C
ATOM    502  CD1  ILE A   64      25.080  47.930   -9.867   1.00  45.66   C
ATOM    503  N    TYR A   65      23.811  42.175  -11.373   1.00  41.50   N
ATOM    504  CA   TYR A   65      23.398  40.851  -10.917   1.00  41.75   C
ATOM    505  C    TYR A   65      24.239  40.399   -9.746   1.00  46.17   C
ATOM    506  O    TYR A   65      25.400  40.796   -9.628   1.00  46.44   O
ATOM    507  CB   TYR A   65      23.591  39.814  -12.023   1.00  39.24   C
ATOM    508  CG   TYR A   65      22.643  39.936  -13.177   1.00  46.02   C
ATOM    509  CD1  TYR A   65      23.074  40.408  -14.415   1.00  43.20   C
ATOM    510  CD2  TYR A   65      21.304  39.560  -13.035   1.00  40.19   C
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Figure 2 (Table 2 (page 17))

ATOM	511	CE1	TYR	A	65	22.198	40.503	-15.492	1.00 46.92	C
ATOM	512	CE2	TYR	A	65	20.406	39.644	-14.117	1.00 42.02	C
ATOM	513	CZ	TYR	A	65	20.868	40.117	-15.337	1.00 47.29	C
ATOM	514	OH	TYR	A	65	20.008	40.185	-16.399	1.00 46.88	O
ATOM	515	N	ASN	A	66	23.660	39.556	-8.897	1.00 43.81	N
ATOM	516	CA	ASN	A	66	24.368	38.990	-7.756	1.00 48.17	C
ATOM	517	C	ASN	A	66	25.277	40.002	-7.062	1.00 48.24	C
ATOM	518	O	ASN	A	66	26.489	39.792	-6.955	1.00 48.04	O
ATOM	519	CB	ASN	A	66	25.206	37.817	-8.241	1.00 44.79	C
ATOM	520	CG	ASN	A	66	25.844	37.052	-7.100	1.00 58.80	C
ATOM	521	OD1	ASN	A	66	26.868	36.393	-7.279	1.00 62.64	O
ATOM	522	ND2	ASN	A	66	25.237	37.127	-5.919	1.00 60.17	N
ATOM	523	N	ALA	A	67	24.684	41.080	-6.566	1.00 47.68	N
ATOM	524	CA	ALA	A	67	25.448	42.151	-5.935	1.00 40.81	C
ATOM	525	C	ALA	A	67	26.301	41.798	-4.739	1.00 49.08	C
ATOM	526	O	ALA	A	67	25.937	40.963	-3.910	1.00 47.57	O
ATOM	527	CB	ALA	A	67	24.523	43.290	-5.553	1.00 44.48	C
ATOM	528	N	ASN	A	68	27.435	42.482	-4.649	1.00 50.95	N
ATOM	529	CA	ASN	A	68	28.344	42.315	-3.529	1.00 54.43	C
ATOM	530	C	ASN	A	68	28.763	43.719	-3.093	1.00 55.80	C
ATOM	531	O	ASN	A	68	28.665	44.678	-3.872	1.00 45.45	O
ATOM	532	CB	ASN	A	68	29.557	41.476	-3.922	1.00 51.73	C
ATOM	533	CG	ASN	A	68	30.494	42.201	-4.854	1.00 61.49	C
ATOM	534	OD1	ASN	A	68	30.920	43.322	-4.579	1.00 60.88	O
ATOM	535	ND2	ASN	A	68	30.835	41.554	-5.963	1.00 52.62	N
ATOM	536	N	ILE	A	69	29.235	43.835	-1.856	1.00 52.73	N
ATOM	537	CA	ILE	A	69	29.630	45.118	-1.285	1.00 58.71	C
ATOM	538	C	ILE	A	69	30.545	45.990	-2.137	1.00 51.79	C
ATOM	539	O	ILE	A	69	30.483	47.208	-2.043	1.00 52.79	O
ATOM	540	CB	ILE	A	69	30.299	44.937	0.095	1.00 60.50	C
ATOM	541	CG1	ILE	A	69	31.681	44.301	-0.063	1.00 67.17	C
ATOM	542	CG2	ILE	A	69	29.410	44.091	0.987	1.00 59.59	C
ATOM	543	CD1	ILE	A	69	32.506	44.314	1.211	1.00 80.29	C
ATOM	544	N	ASP	A	70	31.396	45.384	-2.956	1.00 46.36	N
ATOM	545	CA	ASP	A	70	32.277	46.184	-3.781	1.00 50.45	C
ATOM	546	C	ASP	A	70	31.587	46.792	-4.991	1.00 58.77	C
ATOM	547	O	ASP	A	70	32.227	47.477	-5.784	1.00 53.61	O
ATOM	548	CB	ASP	A	70	33.473	45.369	-4.241	1.00 50.41	C
ATOM	549	CG	ASP	A	70	34.388	44.991	-3.088	1.00 69.82	C
ATOM	550	OD1	ASP	A	70	34.622	45.851	-2.208	1.00 68.65	O
ATOM	551	OD2	ASP	A	70	34.878	43.842	-3.064	1.00 67.67	O
ATOM	552	N	ASP	A	71	30.290	46.540	-5.144	1.00 54.09	N
ATOM	553	CA	ASP	A	71	29.554	47.102	-6.269	1.00 50.10	C
ATOM	554	C	ASP	A	71	28.969	48.474	-5.898	1.00 52.41	C
ATOM	555	O	ASP	A	71	28.508	49.224	-6.764	1.00 47.41	O
ATOM	556	CB	ASP	A	71	28.406	46.166	-6.708	1.00 49.99	C
ATOM	557	CG	ASP	A	71	28.892	44.834	-7.302	1.00 49.02	C
ATOM	558	OD1	ASP	A	71	29.813	44.825	-8.146	1.00 46.46	O
ATOM	559	OD2	ASP	A	71	28.324	43.784	-6.929	1.00 50.74	O
ATOM	560	N	ALA	A	72	28.987	48.801	-4.610	1.00 42.72	N
ATOM	561	CA	ALA	A	72	28.429	50.063	-4.133	1.00 45.31	C
ATOM	562	C	ALA	A	72	29.129	51.291	-4.686	1.00 47.73	C
ATOM	563	O	ALA	A	72	30.326	51.268	-4.977	1.00 47.41	O
ATOM	564	CB	ALA	A	72	28.460	50.107	-2.604	1.00 47.05	C
ATOM	565	N	GLY	A	73	28.378	52.374	-4.821	1.00 48.72	N
ATOM	566	CA	GLY	A	73	28.976	53.593	-5.322	1.00 54.09	C
ATOM	567	C	GLY	A	73	28.144	54.331	-6.341	1.00 51.98	C

Figure 2 (Table 2 (page 18))

ATOM	568	O	GLY A	73	27.018	53.939	-6.653	1.00	49.57	O
ATOM	569	N	ILE A	74	28.716	55.413	-6.859	1.00	51.79	N
ATOM	570	CA	ILE A	74	28.052	56.242	-7.850	1.00	48.58	C
ATOM	571	C	ILE A	74	28.428	55.760	-9.237	1.00	47.75	C
ATOM	572	O	ILE A	74	29.603	55.780	-9.620	1.00	46.87	O
ATOM	573	CB	ILE A	74	28.475	57.717	-7.705	1.00	54.10	C
ATOM	574	CG1	ILE A	74	28.061	58.227	-6.323	1.00	60.29	C
ATOM	575	CG2	ILE A	74	27.860	58.551	-8.816	1.00	51.72	C
ATOM	576	CD1	ILE A	74	28.463	59.656	-6.041	1.00	55.15	C
ATOM	577	N	TYR A	75	27.429	55.272	-9.960	1.00	39.87	N
ATOM	578	CA	TYR A	75	27.637	54.826	-11.330	1.00	48.23	C
ATOM	579	C	TYR A	75	27.168	56.010	-12.126	1.00	48.15	C
ATOM	580	O	TYR A	75	26.293	56.764	-11.682	1.00	46.43	O
ATOM	581	CB	TYR A	75	26.745	53.629	-11.707	1.00	44.56	C
ATOM	582	CG	TYR A	75	27.137	52.331	-11.050	1.00	47.56	C
ATOM	583	CD1	TYR A	75	26.925	52.133	-9.682	1.00	39.03	C
ATOM	584	CD2	TYR A	75	27.789	51.326	-11.773	1.00	43.44	C
ATOM	585	CE1	TYR A	75	27.356	50.967	-9.045	1.00	39.99	C
ATOM	586	CE2	TYR A	75	28.230	50.162	-11.146	1.00	32.79	C
ATOM	587	CZ	TYR A	75	28.010	49.990	-9.778	1.00	35.84	C
ATOM	588	OH	TYR A	75	28.463	48.851	-9.153	1.00	43.95	O
ATOM	589	N	LYS A	76	27.739	56.201	-13.299	1.00	48.85	N
ATOM	590	CA	LYS A	76	27.270	57.305	-14.090	1.00	48.84	C
ATOM	591	C	LYS A	76	27.178	56.938	-15.532	1.00	44.98	C
ATOM	592	O	LYS A	76	27.912	56.092	-16.052	1.00	47.18	O
ATOM	593	CB	LYS A	76	28.115	58.551	-13.857	1.00	56.56	C
ATOM	594	CG	LYS A	76	29.442	58.619	-14.520	1.00	59.09	C
ATOM	595	CD	LYS A	76	30.046	59.941	-14.072	1.00	66.83	C
ATOM	596	CE	LYS A	76	31.142	60.452	-14.968	1.00	71.43	C
ATOM	597	NZ	LYS A	76	31.553	61.794	-14.449	1.00	73.15	N
ATOM	598	N	CYS A	77	26.194	57.553	-16.153	1.00	45.89	N
ATOM	599	CA	CYS A	77	25.888	57.319	-17.532	1.00	44.65	C
ATOM	600	C	CYS A	77	26.233	58.600	-18.270	1.00	47.89	C
ATOM	601	O	CYS A	77	25.718	59.666	-17.945	1.00	52.98	O
ATOM	602	CB	CYS A	77	24.401	57.004	-17.652	1.00	42.61	C
ATOM	603	SG	CYS A	77	23.808	56.802	-19.350	1.00	61.23	S
ATOM	604	N	VAL A	78	27.122	58.494	-19.249	1.00	50.12	N
ATOM	605	CA	VAL A	78	27.547	59.658	-20.019	1.00	46.50	C
ATOM	606	C	VAL A	78	27.082	59.581	-21.471	1.00	43.99	C
ATOM	607	O	VAL A	78	27.222	58.552	-22.131	1.00	48.45	O
ATOM	608	CB	VAL A	78	29.084	59.795	-19.993	1.00	46.58	C
ATOM	609	CG1	VAL A	78	29.517	61.010	-20.820	1.00	51.99	C
ATOM	610	CG2	VAL A	78	29.566	59.942	-18.547	1.00	41.06	C
ATOM	611	N	VAL A	79	26.521	60.672	-21.965	1.00	48.68	N
ATOM	612	CA	VAL A	79	26.047	60.720	-23.343	1.00	57.39	C
ATOM	613	C	VAL A	79	26.945	61.666	-24.119	1.00	54.87	C
ATOM	614	O	VAL A	79	27.194	62.792	-23.691	1.00	52.91	O
ATOM	615	CB	VAL A	79	24.598	61.227	-23.417	1.00	60.20	C
ATOM	616	CG1	VAL A	79	24.085	61.155	-24.848	1.00	54.06	C
ATOM	617	CG2	VAL A	79	23.730	60.395	-22.487	1.00	56.02	C
ATOM	618	N	THR A	80	27.452	61.191	-25.247	1.00	48.32	N
ATOM	619	CA	THR A	80	28.313	62.011	-26.066	1.00	52.81	C
ATOM	620	C	THR A	80	27.706	62.226	-27.450	1.00	54.17	C
ATOM	621	O	THR A	80	27.501	61.266	-28.187	1.00	49.22	O
ATOM	622	CB	THR A	80	29.691	61.371	-26.241	1.00	54.94	C
ATOM	623	OG1	THR A	80	30.268	61.104	-24.954	1.00	54.31	O
ATOM	624	CG2	THR A	80	30.601	62.318	-27.012	1.00	41.33	C

Figure 2 (Table 2 (page 19))

ATOM	625	N	ALA	A	81	27.430	63.487	-27.787	1.00	56.76	N
ATOM	626	CA	ALA	A	81	26.859	63.866	-29.088	1.00	58.85	C
ATOM	627	C	ALA	A	81	27.942	63.828	-30.165	1.00	58.97	C
ATOM	628	O	ALA	A	81	29.131	63.922	-29.847	1.00	53.72	O
ATOM	629	CB	ALA	A	81	26.263	65.265	-29.005	1.00	60.88	C
ATOM	630	N	GLU	A	82	27.528	63.712	-31.429	1.00	67.86	N
ATOM	631	CA	GLU	A	82	28.462	63.639	-32.555	1.00	73.18	C
ATOM	632	C	GLU	A	82	29.599	64.664	-32.507	1.00	68.06	C
ATOM	633	O	GLU	A	82	30.700	64.398	-32.993	1.00	65.36	O
ATOM	634	CB	GLU	A	82	27.707	63.768	-33.887	1.00	74.95	C
ATOM	635	CG	GLU	A	82	28.027	62.638	-34.868	1.00	98.35	C
ATOM	636	CD	GLU	A	82	27.295	62.768	-36.194	1.00	111.66	C
ATOM	637	OE1	GLU	A	82	26.071	63.034	-36.178	1.00	118.11	O
ATOM	638	OE2	GLU	A	82	27.942	62.594	-37.253	1.00	117.01	O
ATOM	639	N	ASP	A	83	29.340	65.821	-31.907	1.00	62.35	N
ATOM	640	CA	ASP	A	83	30.340	66.877	-31.812	1.00	67.89	C
ATOM	641	C	ASP	A	83	31.171	66.830	-30.533	1.00	71.00	C
ATOM	642	O	ASP	A	83	31.929	67.759	-30.246	1.00	73.73	O
ATOM	643	CB	ASP	A	83	29.653	68.230	-31.924	1.00	74.31	C
ATOM	644	CG	ASP	A	83	28.664	68.461	-30.815	1.00	82.18	C
ATOM	645	OD1	ASP	A	83	27.939	67.508	-30.462	1.00	93.75	O
ATOM	646	OD2	ASP	A	83	28.606	69.593	-30.301	1.00	87.77	O
ATOM	647	N	GLY	A	84	31.017	65.760	-29.759	1.00	69.26	N
ATOM	648	CA	GLY	A	84	31.790	65.617	-28.533	1.00	61.95	C
ATOM	649	C	GLY	A	84	31.242	66.254	-27.266	1.00	62.86	C
ATOM	650	O	GLY	A	84	31.851	66.139	-26.197	1.00	65.82	O
ATOM	651	N	THR	A	85	30.106	66.936	-27.361	1.00	55.77	N
ATOM	652	CA	THR	A	85	29.535	67.559	-26.176	1.00	63.65	C
ATOM	653	C	THR	A	85	28.929	66.445	-25.320	1.00	61.95	C
ATOM	654	O	THR	A	85	28.291	65.528	-25.839	1.00	56.86	O
ATOM	655	CB	THR	A	85	28.471	68.614	-26.555	1.00	61.72	C
ATOM	656	OG1	THR	A	85	27.458	68.019	-27.373	1.00	73.83	O
ATOM	657	CG2	THR	A	85	29.125	69.749	-27.325	1.00	69.89	C
ATOM	658	N	GLN	A	86	29.130	66.520	-24.011	1.00	58.16	N
ATOM	659	CA	GLN	A	86	28.628	65.464	-23.141	1.00	63.76	C
ATOM	660	C	GLN	A	86	27.696	65.900	-22.030	1.00	62.47	C
ATOM	661	O	GLN	A	86	27.803	67.011	-21.505	1.00	64.92	O
ATOM	662	CB	GLN	A	86	29.793	64.715	-22.498	1.00	56.96	C
ATOM	663	CG	GLN	A	86	30.860	64.242	-23.460	1.00	50.20	C
ATOM	664	CD	GLN	A	86	31.964	63.519	-22.724	1.00	54.10	C
ATOM	665	OE1	GLN	A	86	32.390	63.965	-21.663	1.00	54.08	O
ATOM	666	NE2	GLN	A	86	32.436	62.401	-23.276	1.00	56.27	N
ATOM	667	N	SER	A	87	26.800	64.986	-21.667	1.00	63.47	N
ATOM	668	CA	SER	A	87	25.836	65.182	-20.588	1.00	68.11	C
ATOM	669	C	SER	A	87	25.889	63.906	-19.749	1.00	65.62	C
ATOM	670	O	SER	A	87	26.194	62.829	-20.270	1.00	69.37	O
ATOM	671	CB	SER	A	87	24.420	65.362	-21.150	1.00	75.52	C
ATOM	672	OG	SER	A	87	24.344	66.449	-22.057	1.00	88.36	O
ATOM	673	N	GLU	A	88	25.592	64.009	-18.460	1.00	63.19	N
ATOM	674	CA	GLU	A	88	25.623	62.827	-17.607	1.00	53.44	C
ATOM	675	C	GLU	A	88	24.532	62.803	-16.556	1.00	59.13	C
ATOM	676	O	GLU	A	88	23.942	63.824	-16.209	1.00	58.88	O
ATOM	677	CB	GLU	A	88	26.976	62.711	-16.904	1.00	60.59	C
ATOM	678	CG	GLU	A	88	27.272	63.816	-15.898	1.00	67.25	C
ATOM	679	CD	GLU	A	88	28.656	63.687	-15.277	1.00	78.40	C
ATOM	680	OE1	GLU	A	88	29.631	63.494	-16.035	1.00	79.36	O
ATOM	681	OE2	GLU	A	88	28.773	63.782	-14.033	1.00	81.96	O

Figure 2 (Table 2 (page 20))

ATOM	682	N	ALA	A	89	24.254	61.602	-16.079	1.00	54.88	N
ATOM	683	CA	ALA	A	89	23.283	61.384	-15.027	1.00	45.50	C
ATOM	684	C	ALA	A	89	24.036	60.407	-14.149	1.00	52.74	C
ATOM	685	O	ALA	A	89	24.777	59.552	-14.659	1.00	48.26	O
ATOM	686	CB	ALA	A	89	22.022	60.736	-15.567	1.00	53.66	C
ATOM	687	N	THR	A	90	23.887	60.549	-12.839	1.00	46.21	N
ATOM	688	CA	THR	A	90	24.558	59.647	-11.932	1.00	49.08	C
ATOM	689	C	THR	A	90	23.515	58.993	-11.051	1.00	49.13	C
ATOM	690	O	THR	A	90	22.402	59.516	-10.861	1.00	49.24	O
ATOM	691	CB	THR	A	90	25.587	60.376	-11.052	1.00	48.30	C
ATOM	692	OG1	THR	A	90	24.932	61.366	-10.256	1.00	53.97	O
ATOM	693	CG2	THR	A	90	26.640	61.041	-11.915	1.00	52.65	C
ATOM	694	N	VAL	A	91	23.871	57.823	-10.539	1.00	45.14	N
ATOM	695	CA	VAL	A	91	22.966	57.102	-9.667	1.00	48.65	C
ATOM	696	C	VAL	A	91	23.736	56.474	-8.527	1.00	45.53	C
ATOM	697	O	VAL	A	91	24.708	55.754	-8.740	1.00	47.93	O
ATOM	698	CB	VAL	A	91	22.164	56.035	-10.433	1.00	50.62	C
ATOM	699	CG1	VAL	A	91	23.113	55.013	-11.094	1.00	48.35	C
ATOM	700	CG2	VAL	A	91	21.177	55.349	-9.474	1.00	54.01	C
ATOM	701	N	ASN	A	92	23.304	56.773	-7.306	1.00	49.96	N
ATOM	702	CA	ASN	A	92	23.964	56.255	-6.116	1.00	50.90	C
ATOM	703	C	ASN	A	92	23.399	54.887	-5.780	1.00	45.05	C
ATOM	704	O	ASN	A	92	22.220	54.742	-5.466	1.00	48.81	O
ATOM	705	CB	ASN	A	92	23.757	57.200	-4.932	1.00	47.93	C
ATOM	706	CG	ASN	A	92	24.569	56.786	-3.724	1.00	54.25	C
ATOM	707	OD1	ASN	A	92	24.115	56.897	-2.584	1.00	56.44	O
ATOM	708	ND2	ASN	A	92	25.784	56.304	-3.969	1.00	54.09	N
ATOM	709	N	VAL	A	93	24.256	53.881	-5.851	1.00	46.44	N
ATOM	710	CA	VAL	A	93	23.831	52.527	-5.574	1.00	47.68	C
ATOM	711	C	VAL	A	93	24.387	52.085	-4.232	1.00	46.87	C
ATOM	712	O	VAL	A	93	25.602	52.009	-4.053	1.00	45.39	O
ATOM	713	CB	VAL	A	93	24.310	51.548	-6.679	1.00	44.88	C
ATOM	714	CG1	VAL	A	93	23.834	50.143	-6.365	1.00	50.34	C
ATOM	715	CG2	VAL	A	93	23.769	51.981	-8.042	1.00	51.13	C
ATOM	716	N	LYS	A	94	23.490	51.807	-3.290	1.00	52.11	N
ATOM	717	CA	LYS	A	94	23.902	51.347	-1.961	1.00	59.43	C
ATOM	718	C	LYS	A	94	23.774	49.832	-1.886	1.00	55.63	C
ATOM	719	O	LYS	A	94	22.871	49.241	-2.471	1.00	43.24	O
ATOM	720	CB	LYS	A	94	23.033	51.960	-0.855	1.00	55.35	C
ATOM	721	CG	LYS	A	94	23.173	53.464	-0.668	1.00	65.17	C
ATOM	722	CD	LYS	A	94	22.156	53.977	0.356	1.00	67.48	C
ATOM	723	CE	LYS	A	94	22.081	55.492	0.362	1.00	74.84	C
ATOM	724	NZ	LYS	A	94	21.040	55.986	1.310	1.00	78.54	N
ATOM	725	N	ILE	A	95	24.699	49.202	-1.181	1.00	56.66	N
ATOM	726	CA	ILE	A	95	24.658	47.762	-1.004	1.00	56.71	C
ATOM	727	C	ILE	A	95	24.467	47.546	0.495	1.00	59.65	C
ATOM	728	O	ILE	A	95	25.004	48.298	1.305	1.00	53.96	O
ATOM	729	CB	ILE	A	95	25.981	47.086	-1.451	1.00	50.11	C
ATOM	730	CG1	ILE	A	95	26.247	47.361	-2.935	1.00	58.21	C
ATOM	731	CG2	ILE	A	95	25.905	45.584	-1.206	1.00	55.81	C
ATOM	732	CD1	ILE	A	95	25.141	46.878	-3.869	1.00	46.59	C
ATOM	733	N	PHE	A	96	23.670	46.553	0.863	1.00	56.77	N
ATOM	734	CA	PHE	A	96	23.464	46.249	2.269	1.00	56.57	C
ATOM	735	C	PHE	A	96	23.070	44.791	2.380	1.00	52.33	C
ATOM	736	O	PHE	A	96	22.921	44.087	1.375	1.00	55.58	O
ATOM	737	CB	PHE	A	96	22.389	47.146	2.893	1.00	51.68	C

Figure 2 (Table 2 (page 21))

ATOM	738	CG	PHE	A	96	20.984	46.731	2.570	1.00 55.80	C
ATOM	739	CD1	PHE	A	96	20.078	46.441	3.589	1.00 56.18	C
ATOM	740	CD2	PHE	A	96	20.565	46.630	1.249	1.00 53.68	C
ATOM	741	CE1	PHE	A	96	18.770	46.055	3.287	1.00 61.36	C
ATOM	742	CE2	PHE	A	96	19.268	46.249	0.932	1.00 54.41	C
ATOM	743	CZ	PHE	A	96	18.362	45.959	1.951	1.00 51.56	C
ATOM	744	N	GLN	A	97	22.929	44.323	3.607	1.00 44.80	N
ATOM	745	CA	GLN	A	97	22.565	42.945	3.819	1.00 41.35	C
ATOM	746	C	GLN	A	97	21.257	42.956	4.559	1.00 43.49	C
ATOM	747	O	GLN	A	97	21.185	43.352	5.725	1.00 48.61	O
ATOM	748	CB	GLN	A	97	23.639	42.220	4.639	1.00 50.03	C
ATOM	749	CG	GLN	A	97	23.239	40.811	5.074	1.00 42.38	C
ATOM	750	CD	GLN	A	97	22.968	39.885	3.899	1.00 45.87	C
ATOM	751	OE1	GLN	A	97	23.879	39.539	3.148	1.00 50.97	O
ATOM	752	NE2	GLN	A	97	21.712	39.485	3.725	1.00 43.50	N
ATOM	753	N	LYS	A	98	20.208	42.557	3.861	1.00 43.56	N
ATOM	754	CA	LYS	A	98	18.914	42.503	4.493	1.00 50.07	C
ATOM	755	C	LYS	A	98	18.988	41.436	5.594	1.00 45.12	C
ATOM	756	O	LYS	A	98	19.772	40.483	5.518	1.00 44.19	O
ATOM	757	CB	LYS	A	98	17.835	42.141	3.467	1.00 42.89	C
ATOM	758	CG	LYS	A	98	17.806	40.689	3.029	1.00 54.06	C
ATOM	759	CD	LYS	A	98	16.620	40.432	2.091	1.00 70.03	C
ATOM	760	CE	LYS	A	98	16.542	38.972	1.674	1.00 74.47	C
ATOM	761	NZ	LYS	A	98	15.366	38.722	0.799	1.00 87.06	N
ATOM	762	N	LEU	A	99	18.187	41.633	6.625	1.00 42.33	N
ATOM	763	CA	LEU	A	99	18.112	40.718	7.743	1.00 48.11	C
ATOM	764	C	LEU	A	99	17.731	39.322	7.271	1.00 51.43	C
ATOM	765	O	LEU	A	99	16.622	39.119	6.784	1.00 54.69	O
ATOM	766	CB	LEU	A	99	17.058	41.223	8.727	1.00 40.97	C
ATOM	767	CG	LEU	A	99	16.874	40.365	9.974	1.00 51.52	C
ATOM	768	CD1	LEU	A	99	18.114	40.494	10.829	1.00 49.68	C
ATOM	769	CD2	LEU	A	99	15.663	40.822	10.765	1.00 51.15	C
ATOM	770	N	MET	A	100	18.643	38.358	7.388	1.00 48.12	N
ATOM	771	CA	MET	A	100	18.321	36.984	6.995	1.00 51.56	C
ATOM	772	C	MET	A	100	19.033	35.977	7.907	1.00 51.77	C
ATOM	773	O	MET	A	100	19.991	36.322	8.621	1.00 39.76	O
ATOM	774	CB	MET	A	100	18.650	36.727	5.512	1.00 61.21	C
ATOM	775	CG	MET	A	100	20.116	36.564	5.166	1.00 69.49	C
ATOM	776	SD	MET	A	100	20.416	36.505	3.372	1.00 84.60	S
ATOM	777	CE	MET	A	100	19.818	34.884	2.949	1.00 92.44	C
ATOM	778	N	PHE	A	101	18.531	34.745	7.908	1.00 45.49	N
ATOM	779	CA	PHE	A	101	19.085	33.684	8.732	1.00 50.26	C
ATOM	780	C	PHE	A	101	20.138	32.893	7.995	1.00 43.40	C
ATOM	781	O	PHE	A	101	19.907	32.400	6.902	1.00 61.65	O
ATOM	782	CB	PHE	A	101	17.969	32.769	9.210	1.00 46.80	C
ATOM	783	CG	PHE	A	101	17.019	33.450	10.137	1.00 46.54	C
ATOM	784	CD1	PHE	A	101	15.900	34.112	9.652	1.00 52.32	C
ATOM	785	CD2	PHE	A	101	17.274	33.488	11.499	1.00 44.46	C
ATOM	786	CE1	PHE	A	101	15.054	34.822	10.516	1.00 43.20	C
ATOM	787	CE2	PHE	A	101	16.441	34.192	12.366	1.00 48.20	C
ATOM	788	CZ	PHE	A	101	15.322	34.858	11.869	1.00 48.40	C
ATOM	789	N	LYS	A	102	21.302	32.771	8.611	1.00 51.46	N
ATOM	790	CA	LYS	A	102	22.420	32.066	8.009	1.00 48.23	C
ATOM	791	C	LYS	A	102	22.516	30.619	8.468	1.00 54.86	C
ATOM	792	O	LYS	A	102	22.768	29.712	7.668	1.00 62.07	O
ATOM	793	CB	LYS	A	102	23.714	32.799	8.340	1.00 57.97	C

Figure 2 (Table 2 (page 22))

ATOM	794	CG	LYS	A	102	24.954	32.199	7.720	1.00 71.82	C
ATOM	795	CD	LYS	A	102	26.170	33.021	8.108	1.00 82.19	C
ATOM	796	CE	LYS	A	102	27.335	32.773	7.169	1.00 88.42	C
ATOM	797	NZ	LYS	A	102	28.516	33.602	7.540	1.00 98.10	N
ATOM	798	N	ASN	A	103	22.328	30.409	9.763	1.00 47.83	N
ATOM	799	CA	ASN	A	103	22.379	29.081	10.339	1.00 43.78	C
ATOM	800	C	ASN	A	103	21.419	29.084	11.525	1.00 45.04	C
ATOM	801	O	ASN	A	103	21.661	29.751	12.534	1.00 40.24	O
ATOM	802	CB	ASN	A	103	23.802	28.764	10.800	1.00 45.29	C
ATOM	803	CG	ASN	A	103	23.886	27.468	11.565	1.00 46.73	C
ATOM	804	OD1	ASN	A	103	23.582	26.402	11.037	1.00 54.61	O
ATOM	805	ND2	ASN	A	103	24.308	27.552	12.822	1.00 50.10	N
ATOM	806	N	ALA	A	104	20.312	28.369	11.379	1.00 40.89	N
ATOM	807	CA	ALA	A	104	19.304	28.264	12.422	1.00 48.41	C
ATOM	808	C	ALA	A	104	18.651	26.906	12.200	1.00 52.07	C
ATOM	809	O	ALA	A	104	17.490	26.811	11.829	1.00 51.94	O
ATOM	810	CB	ALA	A	104	18.280	29.359	12.241	1.00 53.18	C
ATOM	811	N	PRO	A	105	19.386	25.834	12.461	1.00 47.52	N
ATOM	812	CA	PRO	A	105	18.873	24.481	12.265	1.00 45.57	C
ATOM	813	C	PRO	A	105	17.700	24.096	13.112	1.00 47.49	C
ATOM	814	O	PRO	A	105	17.508	24.606	14.223	1.00 41.72	O
ATOM	815	CB	PRO	A	105	20.087	23.588	12.501	1.00 49.47	C
ATOM	816	CG	PRO	A	105	21.055	24.460	13.270	1.00 52.18	C
ATOM	817	CD	PRO	A	105	20.631	25.867	13.230	1.00 52.90	C
ATOM	818	N	THR	A	106	16.864	23.260	12.515	1.00 48.69	N
ATOM	819	CA	THR	A	106	15.717	22.758	13.215	1.00 52.32	C
ATOM	820	C	THR	A	106	15.529	21.322	12.759	1.00 58.90	C
ATOM	821	O	THR	A	106	15.672	20.999	11.581	1.00 55.09	O
ATOM	822	CB	THR	A	106	14.447	23.612	12.955	1.00 53.67	C
ATOM	823	OG1	THR	A	106	13.355	23.053	13.698	1.00 54.59	O
ATOM	824	CG2	THR	A	106	14.097	23.641	11.468	1.00 58.16	C
ATOM	825	N	PRO	A	107	15.275	20.424	13.714	1.00 52.16	N
ATOM	826	CA	PRO	A	107	15.184	20.737	15.138	1.00 43.22	C
ATOM	827	C	PRO	A	107	16.585	20.810	15.732	1.00 47.05	C
ATOM	828	O	PRO	A	107	17.578	20.532	15.064	1.00 45.59	O
ATOM	829	CB	PRO	A	107	14.426	19.539	15.688	1.00 49.39	C
ATOM	830	CG	PRO	A	107	15.052	18.411	14.902	1.00 55.45	C
ATOM	831	CD	PRO	A	107	15.065	18.986	13.480	1.00 55.64	C
ATOM	832	N	GLN	A	108	16.650	21.202	16.994	1.00 40.58	N
ATOM	833	CA	GLN	A	108	17.901	21.229	17.709	1.00 46.97	C
ATOM	834	C	GLN	A	108	17.566	20.339	18.896	1.00 44.47	C
ATOM	835	O	GLN	A	108	16.492	20.467	19.489	1.00 36.69	O
ATOM	836	CB	GLN	A	108	18.271	22.657	18.084	1.00 40.68	C
ATOM	837	CG	GLN	A	108	18.770	23.436	16.846	1.00 37.05	C
ATOM	838	CD	GLN	A	108	19.203	24.847	17.171	1.00 40.43	C
ATOM	839	OE1	GLN	A	108	19.879	25.073	18.172	1.00 36.29	O
ATOM	840	NE2	GLN	A	108	18.828	25.805	16.332	1.00 37.82	N
ATOM	841	N	GLU	A	109	18.469	19.413	19.203	1.00 38.32	N
ATOM	842	CA	GLU	A	109	18.261	18.425	20.257	1.00 39.59	C
ATOM	843	C	GLU	A	109	19.216	18.551	21.424	1.00 44.20	C
ATOM	844	O	GLU	A	109	20.380	18.922	21.254	1.00 41.88	O
ATOM	845	CB	GLU	A	109	18.364	17.033	19.637	1.00 39.87	C
ATOM	846	CG	GLU	A	109	17.437	16.885	18.448	1.00 45.54	C
ATOM	847	CD	GLU	A	109	17.358	15.478	17.912	1.00 49.95	C
ATOM	848	OE1	GLU	A	109	17.335	14.518	18.713	1.00 54.48	O
ATOM	849	OE2	GLU	A	109	17.295	15.330	16.678	1.00 54.37	O

Figure 2 (Table 2 (page 23))

ATOM	850	N	PHE A 110	18.713	18.223	22.609	1.00	36.31	N
ATOM	851	CA	PHE A 110	19.491	18.314	23.825	1.00	37.31	C
ATOM	852	C	PHE A 110	19.154	17.167	24.748	1.00	44.15	C
ATOM	853	O	PHE A 110	18.071	16.596	24.694	1.00	42.74	O
ATOM	854	CB	PHE A 110	19.202	19.643	24.531	1.00	29.73	C
ATOM	855	CG	PHE A 110	19.299	20.831	23.612	1.00	36.45	C
ATOM	856	CD1	PHE A 110	18.189	21.286	22.922	1.00	37.59	C
ATOM	857	CD2	PHE A 110	20.522	21.445	23.387	1.00	35.71	C
ATOM	858	CE1	PHE A 110	18.301	22.337	22.006	1.00	49.86	C
ATOM	859	CE2	PHE A 110	20.649	22.489	22.476	1.00	43.61	C
ATOM	860	CZ	PHE A 110	19.533	22.939	21.785	1.00	39.36	C
ATOM	861	N	LYS A 111	20.108	16.819	25.592	1.00	38.44	N
ATOM	862	CA	LYS A 111	19.909	15.745	26.533	1.00	39.53	C
ATOM	863	C	LYS A 111	19.327	16.395	27.769	1.00	33.66	C
ATOM	864	O	LYS A 111	19.832	17.419	28.238	1.00	37.40	O
ATOM	865	CB	LYS A 111	21.254	15.075	26.845	1.00	35.52	C
ATOM	866	CG	LYS A 111	21.185	13.974	27.890	1.00	45.41	C
ATOM	867	CD	LYS A 111	22.548	13.272	28.006	1.00	51.44	C
ATOM	868	CE	LYS A 111	22.515	12.114	29.000	1.00	58.54	C
ATOM	869	NZ	LYS A 111	23.657	11.172	28.765	1.00	62.26	N
ATOM	870	N	GLU A 112	18.255	15.810	28.287	1.00	39.60	N
ATOM	871	CA	GLU A 112	17.614	16.339	29.478	1.00	42.51	C
ATOM	872	C	GLU A 112	18.627	16.706	30.569	1.00	37.78	C
ATOM	873	O	GLU A 112	19.554	15.950	30.846	1.00	41.69	O
ATOM	874	CB	GLU A 112	16.621	15.312	30.034	1.00	42.05	C
ATOM	875	CG	GLU A 112	15.743	15.888	31.120	1.00	48.02	C
ATOM	876	CD	GLU A 112	14.735	14.886	31.675	1.00	67.88	C
ATOM	877	OE1	GLU A 112	13.582	15.304	31.937	1.00	64.90	O
ATOM	878	OE2	GLU A 112	15.093	13.700	31.865	1.00	70.27	O
ATOM	879	N	GLY A 113	18.448	17.875	31.175	1.00	41.71	N
ATOM	880	CA	GLY A 113	19.350	18.298	32.228	1.00	43.96	C
ATOM	881	C	GLY A 113	20.555	19.128	31.824	1.00	46.88	C
ATOM	882	O	GLY A 113	21.087	19.877	32.652	1.00	44.90	O
ATOM	883	N	GLU A 114	21.017	19.021	30.584	1.00	41.27	N
ATOM	884	CA	GLU A 114	22.181	19.830	30.227	1.00	49.33	C
ATOM	885	C	GLU A 114	21.739	21.260	29.927	1.00	46.85	C
ATOM	886	O	GLU A 114	20.539	21.551	29.864	1.00	45.47	O
ATOM	887	CB	GLU A 114	22.957	19.199	29.052	1.00	46.70	C
ATOM	888	CG	GLU A 114	22.319	19.293	27.682	1.00	49.46	C
ATOM	889	CD	GLU A 114	23.076	18.490	26.613	1.00	56.05	C
ATOM	890	OE1	GLU A 114	24.174	17.946	26.894	1.00	59.22	O
ATOM	891	OE2	GLU A 114	22.565	18.407	25.482	1.00	51.60	O
ATOM	892	N	ASP A 115	22.689	22.181	29.822	1.00	42.06	N
ATOM	893	CA	ASP A 115	22.323	23.554	29.512	1.00	46.33	C
ATOM	894	C	ASP A 115	22.184	23.568	28.018	1.00	46.24	C
ATOM	895	O	ASP A 115	23.107	23.195	27.299	1.00	51.16	O
ATOM	896	CB	ASP A 115	23.394	24.525	29.976	1.00	52.16	C
ATOM	897	CG	ASP A 115	23.530	24.535	31.475	1.00	58.98	C
ATOM	898	OD1	ASP A 115	22.515	24.291	32.169	1.00	56.34	O
ATOM	899	OD2	ASP A 115	24.647	24.785	31.959	1.00	74.61	O
ATOM	900	N	ALA A 116	21.009	23.943	27.536	1.00	40.21	N
ATOM	901	CA	ALA A 116	20.812	23.937	26.105	1.00	41.98	C
ATOM	902	C	ALA A 116	21.024	25.315	25.524	1.00	39.57	C
ATOM	903	O	ALA A 116	20.591	26.311	26.093	1.00	41.84	O
ATOM	904	CB	ALA A 116	19.406	23.428	25.761	1.00	37.59	C
ATOM	905	N	VAL A 117	21.711	25.374	24.396	1.00	35.34	N

Figure 2 (Table 2 (page 24))

ATOM	906	CA	VAL	A	117	21.907	26.651	23.736	1.00 34.85	C
ATOM	907	C	VAL	A	117	21.305	26.459	22.356	1.00 34.14	C
ATOM	908	O	VAL	A	117	21.751	25.608	21.603	1.00 35.50	O
ATOM	909	CB	VAL	A	117	23.391	26.997	23.612	1.00 40.36	C
ATOM	910	CG1	VAL	A	117	23.573	28.240	22.764	1.00 35.45	C
ATOM	911	CG2	VAL	A	117	23.957	27.265	24.994	1.00 46.40	C
ATOM	912	N	ILE	A	118	20.276	27.244	22.046	1.00 35.04	N
ATOM	913	CA	ILE	A	118	19.593	27.169	20.757	1.00 34.21	C
ATOM	914	C	ILE	A	118	20.257	28.172	19.836	1.00 25.24	C
ATOM	915	O	ILE	A	118	20.252	29.371	20.095	1.00 32.78	O
ATOM	916	CB	ILE	A	118	18.106	27.535	20.901	1.00 34.79	C
ATOM	917	CG1	ILE	A	118	17.471	26.651	21.978	1.00 43.37	C
ATOM	918	CG2	ILE	A	118	17.384	27.289	19.578	1.00 35.72	C
ATOM	919	CD1	ILE	A	118	16.071	27.043	22.340	1.00 58.55	C
ATOM	920	N	VAL	A	119	20.829	27.649	18.771	1.00 31.01	N
ATOM	921	CA	VAL	A	119	21.593	28.441	17.830	1.00 37.30	C
ATOM	922	C	VAL	A	119	20.771	29.119	16.753	1.00 37.56	C
ATOM	923	O	VAL	A	119	19.983	28.491	16.065	1.00 40.50	O
ATOM	924	CB	VAL	A	119	22.670	27.549	17.175	1.00 35.82	C
ATOM	925	CG1	VAL	A	119	23.467	28.340	16.136	1.00 34.06	C
ATOM	926	CG2	VAL	A	119	23.582	27.004	18.258	1.00 34.59	C
ATOM	927	N	CYS	A	120	20.980	30.414	16.620	1.00 36.81	N
ATOM	928	CA	CYS	A	120	20.286	31.194	15.610	1.00 32.12	C
ATOM	929	C	CYS	A	120	21.262	32.279	15.148	1.00 33.42	C
ATOM	930	O	CYS	A	120	21.534	33.244	15.873	1.00 34.81	O
ATOM	931	CB	CYS	A	120	19.027	31.819	16.211	1.00 41.13	C
ATOM	932	SG	CYS	A	120	17.972	32.754	15.028	1.00 50.41	S
ATOM	933	N	ASP	A	121	21.821	32.082	13.959	1.00 36.26	N
ATOM	934	CA	ASP	A	121	22.778	33.020	13.370	1.00 38.88	C
ATOM	935	C	ASP	A	121	22.109	33.906	12.333	1.00 36.35	C
ATOM	936	O	ASP	A	121	21.607	33.429	11.326	1.00 41.43	O
ATOM	937	CB	ASP	A	121	23.934	32.251	12.720	1.00 41.76	C
ATOM	938	CG	ASP	A	121	24.766	31.509	13.744	1.00 40.59	C
ATOM	939	OD1	ASP	A	121	25.129	32.153	14.749	1.00 47.54	O
ATOM	940	OD2	ASP	A	121	25.047	30.306	13.560	1.00 45.40	O
ATOM	941	N	VAL	A	122	22.099	35.202	12.584	1.00 41.75	N
ATOM	942	CA	VAL	A	122	21.495	36.119	11.636	1.00 52.79	C
ATOM	943	C	VAL	A	122	22.563	36.999	11.025	1.00 52.22	C
ATOM	944	O	VAL	A	122	23.670	37.115	11.550	1.00 45.91	O
ATOM	945	CB	VAL	A	122	20.458	37.052	12.302	1.00 53.37	C
ATOM	946	CG1	VAL	A	122	19.391	36.242	12.998	1.00 50.48	C
ATOM	947	CG2	VAL	A	122	21.153	37.986	13.275	1.00 58.84	C
ATOM	948	N	VAL	A	123	22.215	37.609	9.901	1.00 47.92	N
ATOM	949	CA	VAL	A	123	23.104	38.525	9.211	1.00 44.45	C
ATOM	950	C	VAL	A	123	22.279	39.739	8.809	1.00 53.24	C
ATOM	951	O	VAL	A	123	21.097	39.610	8.449	1.00 44.25	O
ATOM	952	CB	VAL	A	123	23.713	37.910	7.941	1.00 53.12	C
ATOM	953	CG1	VAL	A	123	24.633	36.758	8.307	1.00 58.99	C
ATOM	954	CG2	VAL	A	123	22.610	37.442	7.012	1.00 54.51	C
ATOM	955	N	SER	A	124	22.911	40.906	8.893	1.00 38.99	N
ATOM	956	CA	SER	A	124	22.304	42.181	8.537	1.00 42.72	C
ATOM	957	C	SER	A	124	23.383	43.252	8.618	1.00 46.36	C
ATOM	958	O	SER	A	124	24.311	43.139	9.420	1.00 48.23	O
ATOM	959	CB	SER	A	124	21.169	42.533	9.496	1.00 45.26	C
ATOM	960	OG	SER	A	124	21.642	42.618	10.828	1.00 50.88	O
ATOM	961	N	SER	A	125	23.257	44.283	7.787	1.00 48.24	N

Figure 2 (Table 2 (page 25))

ATOM	962	CA	SER	A	125	24.221	45.387	7.755	1.00	54.08	C
ATOM	963	C	SER	A	125	24.173	46.098	9.081	1.00	53.53	C
ATOM	964	O	SER	A	125	25.201	46.357	9.694	1.00	54.81	O
ATOM	965	CB	SER	A	125	23.874	46.373	6.641	1.00	45.61	C
ATOM	966	OG	SER	A	125	23.901	45.724	5.391	1.00	46.33	O
ATOM	967	N	LEU	A	126	22.961	46.408	9.519	1.00	51.93	N
ATOM	968	CA	LEU	A	126	22.756	47.077	10.795	1.00	60.20	C
ATOM	969	C	LEU	A	126	22.575	46.030	11.889	1.00	63.51	C
ATOM	970	O	LEU	A	126	22.012	44.961	11.657	1.00	63.28	O
ATOM	971	CB	LEU	A	126	21.521	47.987	10.726	1.00	67.31	C
ATOM	972	CG	LEU	A	126	21.606	49.171	9.746	1.00	75.52	C
ATOM	973	CD1	LEU	A	126	20.323	49.998	9.750	1.00	66.85	C
ATOM	974	CD2	LEU	A	126	22.791	50.045	10.141	1.00	72.14	C
ATOM	975	N	PRO	A	127	23.071	46.308	13.096	1.00	69.25	N
ATOM	976	CA	PRO	A	127	22.925	45.331	14.185	1.00	64.19	C
ATOM	977	C	PRO	A	127	21.463	45.007	14.524	1.00	57.99	C
ATOM	978	O	PRO	A	127	20.655	45.913	14.728	1.00	62.20	O
ATOM	979	CB	PRO	A	127	23.701	45.950	15.354	1.00	64.92	C
ATOM	980	CG	PRO	A	127	23.957	47.367	14.952	1.00	66.17	C
ATOM	981	CD	PRO	A	127	23.849	47.492	13.478	1.00	65.55	C
ATOM	982	N	PRO	A	128	21.126	43.698	14.610	1.00	61.71	N
ATOM	983	CA	PRO	A	128	19.782	43.195	14.906	1.00	61.85	C
ATOM	984	C	PRO	A	128	19.470	43.143	16.362	1.00	62.11	C
ATOM	985	O	PRO	A	128	20.351	42.980	17.192	1.00	64.26	O
ATOM	986	CB	PRO	A	128	19.805	41.776	14.340	1.00	58.63	C
ATOM	987	CG	PRO	A	128	21.070	41.714	13.493	1.00	66.61	C
ATOM	988	CD	PRO	A	128	22.009	42.561	14.287	1.00	51.57	C
ATOM	989	N	THR	A	129	18.196	43.270	16.669	1.00	56.05	N
ATOM	990	CA	THR	A	129	17.759	43.128	18.039	1.00	50.88	C
ATOM	991	C	THR	A	129	17.038	41.791	17.944	1.00	47.70	C
ATOM	992	O	THR	A	129	16.192	41.597	17.072	1.00	52.86	O
ATOM	993	CB	THR	A	129	16.801	44.243	18.457	1.00	59.29	C
ATOM	994	OG1	THR	A	129	17.564	45.360	18.933	1.00	64.98	O
ATOM	995	CG2	THR	A	129	15.885	43.769	19.562	1.00	68.98	C
ATOM	996	N	ILE	A	130	17.377	40.868	18.827	1.00	47.42	N
ATOM	997	CA	ILE	A	130	16.793	39.543	18.779	1.00	49.45	C
ATOM	998	C	ILE	A	130	15.829	39.251	19.914	1.00	48.06	C
ATOM	999	O	ILE	A	130	16.119	39.539	21.074	1.00	49.48	O
ATOM	1000	CB	ILE	A	130	17.907	38.480	18.805	1.00	52.16	C
ATOM	1001	CG1	ILE	A	130	18.711	38.558	17.510	1.00	55.93	C
ATOM	1002	CG2	ILE	A	130	17.317	37.091	19.030	1.00	46.63	C
ATOM	1003	CD1	ILE	A	130	17.934	38.126	16.313	1.00	58.84	C
ATOM	1004	N	ILE	A	131	14.681	38.675	19.568	1.00	45.61	N.
ATOM	1005	CA	ILE	A	131	13.707	38.318	20.588	1.00	50.29	C
ATOM	1006	C	ILE	A	131	13.352	36.859	20.427	1.00	33.83	C
ATOM	1007	O	ILE	A	131	12.993	36.426	19.330	1.00	50.28	O
ATOM	1008	CB	ILE	A	131	12.374	39.104	20.474	1.00	55.23	C
ATOM	1009	CG1	ILE	A	131	12.620	40.610	20.479	1.00	61.34	C
ATOM	1010	CG2	ILE	A	131	11.470	38.737	21.647	1.00	58.84	C
ATOM	1011	CD1	ILE	A	131	12.630	41.236	19.085	1.00	60.34	C
ATOM	1012	N	TRP	A	132	13.437	36.108	21.520	1.00	38.49	N
ATOM	1013	CA	TRP	A	132	13.095	34.692	21.510	1.00	46.49	C
ATOM	1014	C	TRP	A	132	11.668	34.498	22.042	1.00	48.20	C
ATOM	1015	O	TRP	A	132	11.343	34.949	23.133	1.00	45.37	O
ATOM	1016	CB	TRP	A	132	14.085	33.898	22.372	1.00	39.62	C
ATOM	1017	CG	TRP	A	132	15.384	33.632	21.653	1.00	39.42	C

Figure 2 (Table 2 (page 26))

ATOM	1018	CD1	TRP	A	132	16.536	34.369	21.728	1.00	36.55	C
ATOM	1019	CD2	TRP	A	132	15.645	32.570	20.726	1.00	29.03	C
ATOM	1020	NE1	TRP	A	132	17.502	33.826	20.901	1.00	34.64	N
ATOM	1021	CE2	TRP	A	132	16.985	32.725	20.278	1.00	35.20	C
ATOM	1022	CE3	TRP	A	132	14.883	31.502	20.229	1.00	33.72	C
ATOM	1023	CZ2	TRP	A	132	17.572	31.848	19.364	1.00	32.11	C
ATOM	1024	CZ3	TRP	A	132	15.470	30.632	19.318	1.00	35.81	C
ATOM	1025	CH2	TRP	A	132	16.809	30.814	18.893	1.00	33.40	C
ATOM	1026	N	LYS	A	133	10.838	33.809	21.266	1.00	51.27	N
ATOM	1027	CA	LYS	A	133	9.451	33.579	21.645	1.00	57.47	C
ATOM	1028	C	LYS	A	133	9.043	32.124	21.741	1.00	59.45	C
ATOM	1029	O	LYS	A	133	9.408	31.298	20.903	1.00	53.79	O
ATOM	1030	CB	LYS	A	133	8.518	34.267	20.650	1.00	55.78	C
ATOM	1031	CG	LYS	A	133	8.672	35.771	20.593	1.00	66.61	C
ATOM	1032	CD	LYS	A	133	7.816	36.347	19.483	1.00	76.13	C
ATOM	1033	CE	LYS	A	133	7.989	37.857	19.385	1.00	82.76	C
ATOM	1034	NZ	LYS	A	133	7.076	38.469	18.372	1.00	81.20	N
ATOM	1035	N	HIS	A	134	8.274	31.824	22.781	1.00	63.05	N
ATOM	1036	CA	HIS	A	134	7.757	30.481	22.990	1.00	66.48	C
ATOM	1037	C	HIS	A	134	6.265	30.612	23.220	1.00	77.89	C
ATOM	1038	O	HIS	A	134	5.832	31.403	24.067	1.00	63.07	O
ATOM	1039	CB	HIS	A	134	8.370	29.816	24.221	1.00	70.22	C
ATOM	1040	CG	HIS	A	134	8.006	28.368	24.367	1.00	72.09	C
ATOM	1041	ND1	HIS	A	134	8.057	27.704	25.574	1.00	72.16	N
ATOM	1042	CD2	HIS	A	134	7.622	27.448	23.447	1.00	73.41	C
ATOM	1043	CE1	HIS	A	134	7.723	26.440	25.392	1.00	77.82	C
ATOM	1044	NE2	HIS	A	134	7.454	26.257	24.112	1.00	78.13	N
ATOM	1045	N	LYS	A	135	5.488	29.843	22.461	1.00	81.08	N
ATOM	1046	CA	LYS	A	135	4.034	29.850	22.574	1.00	91.79	C
ATOM	1047	C	LYS	A	135	3.435	31.264	22.532	1.00	92.61	C
ATOM	1048	O	LYS	A	135	2.397	31.511	23.139	1.00	95.56	O
ATOM	1049	CB	LYS	A	135	3.608	29.135	23.870	1.00	90.50	C
ATOM	1050	CG	LYS	A	135	3.832	29.955	25.143	1.00	96.62	C
ATOM	1051	CD	LYS	A	135	3.541	29.173	26.414	1.00	94.31	C
ATOM	1052	CE	LYS	A	135	3.714	30.058	27.643	1.00	94.84	C
ATOM	1053	NZ	LYS	A	135	3.553	29.294	28.915	1.00	95.67	N
ATOM	1054	N	GLY	A	136	4.082	32.194	21.828	1.00	91.50	N
ATOM	1055	CA	GLY	A	136	3.553	33.551	21.741	1.00	88.54	C
ATOM	1056	C	GLY	A	136	4.256	34.597	22.589	1.00	85.72	C
ATOM	1057	O	GLY	A	136	4.366	35.754	22.187	1.00	89.77	O
ATOM	1058	N	ARG	A	137	4.734	34.184	23.757	1.00	82.42	N
ATOM	1059	CA	ARG	A	137	5.426	35.064	24.698	1.00	83.81	C
ATOM	1060	C	ARG	A	137	6.867	35.398	24.329	1.00	80.74	C
ATOM	1061	O	ARG	A	137	7.372	35.029	23.272	1.00	83.63	O
ATOM	1062	CB	ARG	A	137	5.448	34.419	26.090	1.00	90.23	C
ATOM	1063	CG	ARG	A	137	4.111	34.360	26.790	1.00	99.62	C
ATOM	1064	CD	ARG	A	137	3.856	35.652	27.530	1.00	105.25	C
ATOM	1065	NE	ARG	A	137	2.445	36.009	27.526	1.00	113.79	N
ATOM	1066	CZ	ARG	A	137	1.973	37.181	27.937	1.00	114.75	C
ATOM	1067	NH1	ARG	A	137	2.805	38.109	28.390	1.00	116.01	N
ATOM	1068	NH2	ARG	A	137	0.672	37.432	27.883	1.00	117.60	N
ATOM	1069	N	ASP	A	138	7.510	36.116	25.241	1.00	76.46	N
ATOM	1070	CA	ASP	A	138	8.907	36.497	25.132	1.00	75.03	C
ATOM	1071	C	ASP	A	138	9.464	35.773	26.328	1.00	76.03	C
ATOM	1072	O	ASP	A	138	9.139	36.102	27.476	1.00	73.85	O
ATOM	1073	CB	ASP	A	138	9.107	38.000	25.318	1.00	77.22	C

Figure 2 (Table 2 (page 27))

```
ATOM   1074  CG   ASP A 138    10.578  38.403  25.275  1.00 77.41 C
ATOM   1075  OD1  ASP A 138    11.410  37.736  25.931  1.00 76.27 O
ATOM   1076  OD2  ASP A 138    10.906  39.394  24.590  1.00 67.17 O
ATOM   1077  N    VAL A 139    10.292  34.776  26.069  1.00 63.30 N
ATOM   1078  CA   VAL A 139    10.838  33.992  27.152  1.00 58.22 C
ATOM   1079  C    VAL A 139    11.541  34.814  28.224  1.00 60.55 C
ATOM   1080  O    VAL A 139    11.799  34.320  29.321  1.00 71.06 O
ATOM   1081  CB   VAL A 139    11.785  32.935  26.595  1.00 62.13 C
ATOM   1082  CG1  VAL A 139    11.091  32.195  25.469  1.00 55.43 C
ATOM   1083  CG2  VAL A 139    13.068  33.588  26.091  1.00 47.09 C
ATOM   1084  N    ILE A 140    11.841  36.070  27.918  1.00 66.18 N
ATOM   1085  CA   ILE A 140    12.519  36.924  28.878  1.00 73.19 C
ATOM   1086  C    ILE A 140    11.594  37.514  29.925  1.00 77.32 C
ATOM   1087  O    ILE A 140    11.822  37.370  31.123  1.00 79.51 O
ATOM   1088  CB   ILE A 140    13.229  38.098  28.183  1.00 75.30 C
ATOM   1089  CG1  ILE A 140    14.357  37.569  27.300  1.00 79.57 C
ATOM   1090  CG2  ILE A 140    13.789  39.062  29.227  1.00 84.41 C
ATOM   1091  CD1  ILE A 140    15.381  36.752  28.065  1.00 75.80 C
ATOM   1092  N    LEU A 141    10.553  38.194  29.468  1.00 85.78 N
ATOM   1093  CA   LEU A 141     9.632  38.838  30.384  1.00 97.07 C
ATOM   1094  C    LEU A 141     8.966  37.937  31.409  1.00101.56 C
ATOM   1095  O    LEU A 141     8.177  38.408  32.225  1.00107.39 O
ATOM   1096  CB   LEU A 141     8.571  39.615  29.608  1.00101.80 C
ATOM   1097  CG   LEU A 141     9.106  40.905  28.991  1.00106.45 C
ATOM   1098  CD1  LEU A 141     7.949  41.736  28.461  1.00108.62 C
ATOM   1099  CD2  LEU A 141     9.882  41.699  30.046  1.00104.45 C
ATOM   1100  N    LYS A 142     9.276  36.650  31.384  1.00101.47 N
ATOM   1101  CA   LYS A 142     8.689  35.751  32.362  1.00101.64 C
ATOM   1102  C    LYS A 142     9.660  35.560  33.527  1.00101.85 C
ATOM   1103  O    LYS A 142     9.262  35.339  34.675  1.00105.32 O
ATOM   1104  CB   LYS A 142     8.346  34.404  31.702  1.00100.75 C
ATOM   1105  CG   LYS A 142     9.525  33.643  31.098  1.00 98.61 C
ATOM   1106  CD   LYS A 142     8.997  32.520  30.208  1.00 93.54 C
ATOM   1107  CE   LYS A 142    10.082  31.550  29.747  1.00 96.37 C
ATOM   1108  NZ   LYS A 142     9.503  30.522  28.822  1.00 91.06 N
ATOM   1109  N    LYS A 143    10.940  35.703  33.223  1.00102.59 N
ATOM   1110  CA   LYS A 143    11.992  35.519  34.206  1.00104.90 C
ATOM   1111  C    LYS A 143    11.852  34.206  34.942  1.00100.79 C
ATOM   1112  O    LYS A 143    11.372  34.122  36.080  1.00100.29 O
ATOM   1113  CB   LYS A 143    12.059  36.672  35.207  1.00107.17 C
ATOM   1114  CG   LYS A 143    13.224  36.510  36.183  1.00113.10 C
ATOM   1115  CD   LYS A 143    14.559  36.248  35.522  1.00116.78 C
ATOM   1116  CE   LYS A 143    15.786  36.228  36.466  1.00123.03 C
ATOM   1117  NZ   LYS A 143    17.123  36.187  35.780  1.00119.60 N
ATOM   1118  N    ASP A 144    12.237  33.182  34.199  1.00 94.81 N
ATOM   1119  CA   ASP A 144    12.319  31.828  34.669  1.00 85.45 C
ATOM   1120  C    ASP A 144    13.827  31.840  34.531  1.00 79.96 C
ATOM   1121  O    ASP A 144    14.365  31.687  33.436  1.00 88.63 O
ATOM   1122  CB   ASP A 144    11.718  30.833  33.677  1.00 85.69 C
ATOM   1123  CG   ASP A 144    11.884  29.398  34.137  1.00 89.87 C
ATOM   1124  OD1  ASP A 144    12.989  29.060  34.609  1.00 90.66 O
ATOM   1125  OD2  ASP A 144    10.913  28.608  34.041  1.00101.36 O
ATOM   1126  N    VAL A 145    14.490  32.118  35.642  1.00 68.69 N
ATOM   1127  CA   VAL A 145    15.946  32.226  35.721  1.00 67.87 C
ATOM   1128  C    VAL A 145    16.758  31.316  34.795  1.00 55.99 C
ATOM   1129  O    VAL A 145    17.915  31.598  34.490  1.00 61.04 O
```

Figure 2 (Table 2 (page 28))

ATOM	1130	CB	VAL	A	145	16.415	31.974	37.167	1.00	76.83	C
ATOM	1131	CG1	VAL	A	145	15.901	33.082	38.076	1.00	76.29	C
ATOM	1132	CG2	VAL	A	145	15.902	30.617	37.655	1.00	77.74	C
ATOM	1133	N	ARG	A	146	16.148	30.227	34.349	1.00	52.68	N
ATOM	1134	CA	ARG	A	146	16.839	29.283	33.493	1.00	56.85	C
ATOM	1135	C	ARG	A	146	16.984	29.771	32.055	1.00	48.40	C
ATOM	1136	O	ARG	A	146	17.808	29.258	31.311	1.00	46.31	O
ATOM	1137	CB	ARG	A	146	16.121	27.925	33.538	1.00	44.42	C
ATOM	1138	CG	ARG	A	146	16.235	27.242	34.901	1.00	53.27	C
ATOM	1139	CD	ARG	A	146	15.613	25.846	34.911	1.00	47.00	C
ATOM	1140	NE	ARG	A	146	14.253	25.864	34.388	1.00	43.57	N
ATOM	1141	CZ	ARG	A	146	13.898	25.279	33.253	1.00	53.19	C
ATOM	1142	NH1	ARG	A	146	14.810	24.627	32.533	1.00	46.06	N
ATOM	1143	NH2	ARG	A	146	12.646	25.359	32.825	1.00	49.59	N
ATOM	1144	N	PHE	A	147	16.190	30.766	31.680	1.00	49.96	N
ATOM	1145	CA	PHE	A	147	16.233	31.297	30.330	1.00	55.08	C
ATOM	1146	C	PHE	A	147	17.068	32.568	30.213	1.00	55.40	C
ATOM	1147	O	PHE	A	147	16.837	33.551	30.916	1.00	58.84	O
ATOM	1148	CB	PHE	A	147	14.815	31.536	29.828	1.00	47.49	C
ATOM	1149	CG	PHE	A	147	14.003	30.271	29.679	1.00	55.00	C
ATOM	1150	CD1	PHE	A	147	13.520	29.598	30.796	1.00	50.35	C
ATOM	1151	CD2	PHE	A	147	13.730	29.747	28.416	1.00	49.95	C
ATOM	1152	CE1	PHE	A	147	12.773	28.416	30.654	1.00	61.13	C
ATOM	1153	CE2	PHE	A	147	12.986	28.571	28.265	1.00	53.83	C
ATOM	1154	CZ	PHE	A	147	12.508	27.905	29.386	1.00	56.75	C
ATOM	1155	N	ILE	A	148	18.038	32.536	29.307	1.00	50.18	N
ATOM	1156	CA	ILE	A	148	18.940	33.661	29.097	1.00	53.42	C
ATOM	1157	C	ILE	A	148	19.348	33.856	27.636	1.00	45.25	C
ATOM	1158	O	ILE	A	148	19.659	32.899	26.944	1.00	44.46	O
ATOM	1159	CB	ILE	A	148	20.233	33.463	29.908	1.00	55.88	C
ATOM	1160	CG1	ILE	A	148	19.907	33.427	31.399	1.00	65.94	C
ATOM	1161	CG2	ILE	A	148	21.231	34.573	29.597	1.00	61.53	C
ATOM	1162	CD1	ILE	A	148	21.093	33.081	32.279	1.00	69.07	C
ATOM	1163	N	VAL	A	149	19.337	35.099	27.172	1.00	37.73	N
ATOM	1164	CA	VAL	A	149	19.764	35.381	25.817	1.00	42.64	C
ATOM	1165	C	VAL	A	149	21.236	35.794	25.962	1.00	46.84	C
ATOM	1166	O	VAL	A	149	21.552	36.756	26.655	1.00	47.29	O
ATOM	1167	CB	VAL	A	149	18.929	36.512	25.185	1.00	42.61	C
ATOM	1168	CG1	VAL	A	149	19.472	36.844	23.791	1.00	44.21	C
ATOM	1169	CG2	VAL	A	149	17.444	36.067	25.064	1.00	43.57	C
ATOM	1170	N	LEU	A	150	22.127	35.036	25.328	1.00	40.34	N
ATOM	1171	CA	LEU	A	150	23.568	35.289	25.400	1.00	42.16	C
ATOM	1172	C	LEU	A	150	24.030	36.450	24.524	1.00	47.24	C
ATOM	1173	O	LEU	A	150	23.262	36.965	23.723	1.00	39.70	O
ATOM	1174	CB	LEU	A	150	24.305	34.019	25.001	1.00	36.82	C
ATOM	1175	CG	LEU	A	150	23.885	32.825	25.860	1.00	50.79	C
ATOM	1176	CD1	LEU	A	150	24.330	31.505	25.225	1.00	45.07	C
ATOM	1177	CD2	LEU	A	150	24.473	32.999	27.252	1.00	55.15	C
ATOM	1178	N	SER	A	151	25.295	36.849	24.666	1.00	50.63	N
ATOM	1179	CA	SER	A	151	25.849	37.953	23.880	1.00	44.74	C
ATOM	1180	C	SER	A	151	25.770	37.710	22.365	1.00	37.06	C
ATOM	1181	O	SER	A	151	25.651	38.663	21.587	1.00	49.84	O
ATOM	1182	CB	SER	A	151	27.320	38.200	24.273	1.00	45.09	C
ATOM	1183	OG	SER	A	151	28.150	37.144	23.792	1.00	45.86	O
ATOM	1184	N	ASN	A	152	25.866	36.455	21.937	1.00	38.65	N
ATOM	1185	CA	ASN	A	152	25.784	36.140	20.506	1.00	40.49	C

Figure 2 (Table 2 (page 29))

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ATOM   1186  C   ASN A 152    24.321  35.998  20.073  1.00  40.22  C
ATOM   1187  O   ASN A 152    24.036  35.583  18.936  1.00  34.75  O
ATOM   1188  CB  ASN A 152    26.476  34.821  20.207  1.00  39.82  C
ATOM   1189  CG  ASN A 152    26.097  33.752  21.199  1.00  54.90  C
ATOM   1190  OD1 ASN A 152    24.972  33.739  21.694  1.00  45.34  O
ATOM   1191  ND2 ASN A 152    27.029  32.850  21.504  1.00  46.13  N
ATOM   1192  N   ASN A 153    23.410  36.309  20.990  1.00  38.94  N
ATOM   1193  CA  ASN A 153    21.969  36.213  20.740  1.00  45.44  C
ATOM   1194  C   ASN A 153    21.352  34.827  20.723  1.00  42.99  C
ATOM   1195  O   ASN A 153    20.171  34.674  20.414  1.00  38.19  O
ATOM   1196  CB  ASN A 153    21.589  36.964  19.469  1.00  42.88  C
ATOM   1197  CG  ASN A 153    21.665  38.468  19.660  1.00  49.74  C
ATOM   1198  OD1 ASN A 153    21.300  38.990  20.720  1.00  57.35  O
ATOM   1199  ND2 ASN A 153    22.130  39.171  18.645  1.00  53.13  N
ATOM   1200  N   TYR A 154    22.121  33.810  21.080  1.00  31.78  N
ATOM   1201  CA  TYR A 154    21.563  32.463  21.151  1.00  37.05  C
ATOM   1202  C   TYR A 154    20.707  32.352  22.418  1.00  36.11  C
ATOM   1203  O   TYR A 154    20.918  33.107  23.357  1.00  35.56  O
ATOM   1204  CB  TYR A 154    22.675  31.425  21.247  1.00  35.50  C
ATOM   1205  CG  TYR A 154    23.535  31.329  20.021  1.00  40.10  C
ATOM   1206  CD1 TYR A 154    24.703  30.565  20.037  1.00  33.69  C
ATOM   1207  CD2 TYR A 154    23.179  31.990  18.837  1.00  35.06  C
ATOM   1208  CE1 TYR A 154    25.505  30.457  18.899  1.00  38.35  C
ATOM   1209  CE2 TYR A 154    23.979  31.892  17.676  1.00  34.58  C
ATOM   1210  CZ  TYR A 154    25.143  31.119  17.726  1.00  46.30  C
ATOM   1211  OH  TYR A 154    25.954  31.005  16.618  1.00  43.90  O
ATOM   1212  N   LEU A 155    19.757  31.415  22.450  1.00  37.10  N
ATOM   1213  CA  LEU A 155    18.936  31.237  23.650  1.00  33.06  C
ATOM   1214  C   LEU A 155    19.514  30.121  24.496  1.00  25.37  C
ATOM   1215  O   LEU A 155    19.688  28.989  24.037  1.00  33.57  O
ATOM   1216  CB  LEU A 155    17.482  30.866  23.303  1.00  33.13  C
ATOM   1217  CG  LEU A 155    16.635  30.561  24.545  1.00  39.86  C
ATOM   1218  CD1 LEU A 155    16.673  31.752  25.480  1.00  39.38  C
ATOM   1219  CD2 LEU A 155    15.185  30.269  24.142  1.00  35.14  C
ATOM   1220  N   GLN A 156    19.802  30.437  25.746  1.00  34.79  N
ATOM   1221  CA  GLN A 156    20.327  29.432  26.638  1.00  30.99  C
ATOM   1222  C   GLN A 156    19.212  28.964  27.568  1.00  33.82  C
ATOM   1223  O   GLN A 156    18.545  29.792  28.205  1.00  38.51  O
ATOM   1224  CB  GLN A 156    21.454  30.010  27.507  1.00  36.98  C
ATOM   1225  CG  GLN A 156    22.028  28.974  28.478  1.00  52.10  C
ATOM   1226  CD  GLN A 156    23.034  29.556  29.461  1.00  59.17  C
ATOM   1227  OE1 GLN A 156    22.750  30.542  30.134  1.00  58.98  O
ATOM   1228  NE2 GLN A 156    24.207  28.934  29.558  1.00  56.95  N
ATOM   1229  N   ILE A 157    19.012  27.651  27.655  1.00  35.15  N
ATOM   1230  CA  ILE A 157    18.001  27.104  28.570  1.00  39.14  C
ATOM   1231  C   ILE A 157    18.737  26.177  29.530  1.00  40.54  C
ATOM   1232  O   ILE A 157    19.028  25.030  29.189  1.00  41.38  O
ATOM   1233  CB  ILE A 157    16.928  26.304  27.832  1.00  36.32  C
ATOM   1234  CG1 ILE A 157    16.195  27.208  26.843  1.00  32.60  C
ATOM   1235  CG2 ILE A 157    15.943  25.728  28.842  1.00  42.84  C
ATOM   1236  CD1 ILE A 157    15.181  26.458  25.983  1.00  40.70  C
ATOM   1237  N   ARG A 158    19.068  26.674  30.718  1.00  38.99  N
ATOM   1238  CA  ARG A 158    19.804  25.857  31.673  1.00  45.51  C
ATOM   1239  C   ARG A 158    18.982  24.711  32.273  1.00  43.75  C
ATOM   1240  O   ARG A 158    17.781  24.851  32.484  1.00  47.32  O
ATOM   1241  CB  ARG A 158    20.381  26.749  32.778  1.00  53.96  C
```

Figure 2 (Table 2 (page 30))

ATOM	1242	CG	ARG	A	158	21.475	27.697	32.272	1.00 70.32	C
ATOM	1243	CD	ARG	A	158	22.155	28.453	33.405	1.00 65.23	C
ATOM	1244	NE	ARG	A	158	21.287	29.449	34.012	1.00 68.48	N
ATOM	1245	CZ	ARG	A	158	21.572	30.079	35.147	1.00 75.70	C
ATOM	1246	NH1	ARG	A	158	22.704	29.808	35.792	1.00 65.00	N
ATOM	1247	NH2	ARG	A	158	20.724	30.973	35.641	1.00 71.67	N
ATOM	1248	N	GLY	A	159	19.653	23.589	32.544	1.00 47.20	N
ATOM	1249	CA	GLY	A	159	18.998	22.415	33.096	1.00 48.68	C
ATOM	1250	C	GLY	A	159	17.731	22.133	32.317	1.00 50.27	C
ATOM	1251	O	GLY	A	159	16.658	21.983	32.897	1.00 44.17	O
ATOM	1252	N	ILE	A	160	17.847	22.050	30.997	1.00 46.11	N
ATOM	1253	CA	ILE	A	160	16.664	21.831	30.189	1.00 39.12	C
ATOM	1254	C	ILE	A	160	15.872	20.590	30.606	1.00 46.02	C
ATOM	1255	O	ILE	A	160	16.434	19.514	30.840	1.00 35.03	O
ATOM	1256	CB	ILE	A	160	17.013	21.755	28.702	1.00 34.52	C
ATOM	1257	CG1	ILE	A	160	15.727	21.917	27.874	1.00 37.12	C
ATOM	1258	CG2	ILE	A	160	17.679	20.446	28.376	1.00 34.14	C
ATOM	1259	CD1	ILE	A	160	15.993	22.199	26.392	1.00 28.22	C
ATOM	1260	N	LYS	A	161	14.557	20.767	30.692	1.00 42.18	N
ATOM	1261	CA	LYS	A	161	13.631	19.710	31.089	1.00 47.02	C
ATOM	1262	C	LYS	A	161	12.855	19.202	29.899	1.00 43.66	C
ATOM	1263	O	LYS	A	161	12.686	19.908	28.899	1.00 41.53	O
ATOM	1264	CB	LYS	A	161	12.599	20.236	32.095	1.00 49.68	C
ATOM	1265	CG	LYS	A	161	13.156	20.896	33.337	1.00 55.48	C
ATOM	1266	CD	LYS	A	161	12.002	21.450	34.178	1.00 65.12	C
ATOM	1267	CE	LYS	A	161	12.488	22.175	35.421	1.00 70.60	C
ATOM	1268	NZ	LYS	A	161	11.350	22.563	36.307	1.00 76.58	N
ATOM	1269	N	LYS	A	162	12.353	17.982	30.020	1.00 44.57	N
ATOM	1270	CA	LYS	A	162	11.560	17.383	28.956	1.00 47.82	C
ATOM	1271	C	LYS	A	162	10.372	18.311	28.670	1.00 43.43	C
ATOM	1272	O	LYS	A	162	9.914	18.427	27.535	1.00 44.67	O
ATOM	1273	CB	LYS	A	162	11.084	15.987	29.391	1.00 50.56	C
ATOM	1274	CG	LYS	A	162	10.298	15.208	28.339	1.00 50.30	C
ATOM	1275	CD	LYS	A	162	11.109	14.958	27.085	1.00 52.43	C
ATOM	1276	CE	LYS	A	162	10.279	14.227	26.051	1.00 60.58	C
ATOM	1277	NZ	LYS	A	162	10.963	14.149	24.731	1.00 59.55	N
ATOM	1278	N	THR	A	163	9.897	19.010	29.691	1.00 44.12	N
ATOM	1279	CA	THR	A	163	8.764	19.904	29.487	1.00 53.06	C
ATOM	1280	C	THR	A	163	9.140	21.234	28.833	1.00 55.60	C
ATOM	1281	O	THR	A	163	8.294	22.107	28.676	1.00 50.18	O
ATOM	1282	CB	THR	A	163	8.022	20.195	30.812	1.00 53.57	C
ATOM	1283	OG1	THR	A	163	8.942	20.712	31.780	1.00 55.40	O
ATOM	1284	CG2	THR	A	163	7.372	18.914	31.349	1.00 55.53	C
ATOM	1285	N	ASP	A	164	10.407	21.397	28.465	1.00 48.62	N
ATOM	1286	CA	ASP	A	164	10.826	22.628	27.810	1.00 42.03	C
ATOM	1287	C	ASP	A	164	10.764	22.477	26.299	1.00 44.90	C
ATOM	1288	O	ASP	A	164	10.821	23.470	25.573	1.00 48.57	O
ATOM	1289	CB	ASP	A	164	12.260	23.017	28.209	1.00 38.06	C
ATOM	1290	CG	ASP	A	164	12.358	23.525	29.631	1.00 36.69	C
ATOM	1291	OD1	ASP	A	164	11.469	24.295	30.052	1.00 49.63	O
ATOM	1292	OD2	ASP	A	164	13.337	23.168	30.327	1.00 44.71	O
ATOM	1293	N	GLU	A	165	10.639	21.251	25.798	1.00 44.64	N
ATOM	1294	CA	GLU	A	165	10.602	21.116	24.353	1.00 53.09	C
ATOM	1295	C	GLU	A	165	9.396	21.821	23.739	1.00 49.63	C
ATOM	1296	O	GLU	A	165	8.465	22.215	24.440	1.00 52.65	O
ATOM	1297	CB	GLU	A	165	10.681	19.650	23.909	1.00 50.75	C

Figure 2 (Table 2 (page 31))

ATOM	1298	CG	GLU A 165	9.828	18.702	24.683	1.00	65.76	C
ATOM	1299	CD	GLU A 165	9.940	17.283	24.155	1.00	72.74	C
ATOM	1300	OE1	GLU A 165	11.040	16.884	23.691	1.00	69.18	O
ATOM	1301	OE2	GLU A 165	8.922	16.565	24.220	1.00	65.52	O
ATOM	1302	N	GLY A 166	9.451	22.002	22.424	1.00	48.94	N
ATOM	1303	CA	GLY A 166	8.405	22.700	21.701	1.00	55.73	C
ATOM	1304	C	GLY A 166	9.067	23.579	20.655	1.00	47.37	C
ATOM	1305	O	GLY A 166	10.256	23.419	20.340	1.00	47.39	O
ATOM	1306	N	THR A 167	8.317	24.517	20.112	0.50	34.99	N
ATOM	1307	CA	THR A 167	8.865	25.386	19.099	0.50	35.61	C
ATOM	1308	C	THR A 167	9.253	26.706	19.720	0.50	31.90	C
ATOM	1309	O	THR A 167	8.524	27.264	20.526	0.50	30.91	O
ATOM	1310	CB	THR A 167	7.849	25.623	18.006	0.50	40.53	C
ATOM	1311	OG1	THR A 167	6.633	26.081	18.602	0.50	51.84	O
ATOM	1312	CG2	THR A 167	7.574	24.332	17.258	0.50	26.00	C
ATOM	1313	N	TYR A 168	10.434	27.191	19.360	1.00	43.71	N
ATOM	1314	CA	TYR A 168	10.922	28.467	19.871	1.00	42.97	C
ATOM	1315	C	TYR A 168	11.183	29.372	18.689	1.00	38.98	C
ATOM	1316	O	TYR A 168	11.801	28.965	17.705	1.00	43.48	O
ATOM	1317	CB	TYR A 168	12.205	28.283	20.682	1.00	44.02	C
ATOM	1318	CG	TYR A 168	11.968	27.702	22.047	1.00	36.86	C
ATOM	1319	CD1	TYR A 168	11.676	26.353	22.206	1.00	38.88	C
ATOM	1320	CD2	TYR A 168	12.000	28.512	23.179	1.00	36.72	C
ATOM	1321	CE1	TYR A 168	11.419	25.821	23.466	1.00	41.93	C
ATOM	1322	CE2	TYR A 168	11.739	27.997	24.440	1.00	42.88	C
ATOM	1323	CZ	TYR A 168	11.451	26.652	24.576	1.00	43.41	C
ATOM	1324	OH	TYR A 168	11.193	26.139	25.824	1.00	40.88	O
ATOM	1325	N	ARG A 169	10.715	30.610	18.787	1.00	44.05	N
ATOM	1326	CA	ARG A 169	10.871	31.533	17.681	1.00	41.18	C
ATOM	1327	C	ARG A 169	12.013	32.526	17.868	1.00	36.73	C
ATOM	1328	O	ARG A 169	12.102	33.216	18.877	1.00	40.52	O
ATOM	1329	CB	ARG A 169	9.552	32.289	17.444	1.00	50.40	C
ATOM	1330	CG	ARG A 169	9.655	33.416	16.430	1.00	60.69	C
ATOM	1331	CD	ARG A 169	8.284	33.861	15.925	1.00	46.23	C
ATOM	1332	NE	ARG A 169	7.716	32.865	15.022	1.00	56.58	N
ATOM	1333	CZ	ARG A 169	6.535	32.984	14.420	1.00	71.77	C
ATOM	1334	NH1	ARG A 169	5.785	34.064	14.621	1.00	58.65	N
ATOM	1335	NH2	ARG A 169	6.101	32.015	13.618	1.00	59.89	N
ATOM	1336	N	CYS A 170	12.888	32.576	16.875	1.00	42.37	N
ATOM	1337	CA	CYS A 170	13.998	33.506	16.919	1.00	45.65	C
ATOM	1338	C	CYS A 170	13.546	34.667	16.025	1.00	31.99	C
ATOM	1339	O	CYS A 170	13.423	34.505	14.810	1.00	41.21	O
ATOM	1340	CB	CYS A 170	15.253	32.840	16.357	1.00	42.01	C
ATOM	1341	SG	CYS A 170	16.748	33.898	16.241	1.00	52.42	S
ATOM	1342	N	GLU A 171	13.289	35.820	16.635	1.00	44.29	N
ATOM	1343	CA	GLU A 171	12.830	36.978	15.879	1.00	49.65	C
ATOM	1344	C	GLU A 171	13.814	38.129	15.844	1.00	40.68	C
ATOM	1345	O	GLU A 171	14.218	38.663	16.885	1.00	45.31	O
ATOM	1346	CB	GLU A 171	11.503	37.502	16.426	1.00	47.28	C
ATOM	1347	CG	GLU A 171	10.905	38.616	15.560	1.00	57.47	C
ATOM	1348	CD	GLU A 171	9.580	39.147	16.096	1.00	65.00	C
ATOM	1349	OE1	GLU A 171	9.593	39.989	17.028	1.00	62.15	O
ATOM	1350	OE2	GLU A 171	8.531	38.707	15.584	1.00	54.66	O
ATOM	1351	N	GLY A 172	14.163	38.525	14.625	1.00	46.09	N
ATOM	1352	CA	GLY A 172	15.086	39.624	14.436	1.00	49.63	C
ATOM	1353	C	GLY A 172	14.388	40.872	13.930	1.00	46.92	C

Figure 2 (Table 2 (page 32))

ATOM	1354	O	GLY	A	172	13.557	40.812	13.014	1.00	50.71	O
ATOM	1355	N	ARG	A	173	14.753	41.998	14.535	1.00	40.06	N
ATOM	1356	CA	ARG	A	173	14.222	43.309	14.215	1.00	44.00	C
ATOM	1357	C	ARG	A	173	15.335	44.350	14.038	1.00	56.42	C
ATOM	1358	O	ARG	A	173	16.328	44.354	14.768	1.00	47.64	O
ATOM	1359	CB	ARG	A	173	13.310	43.800	15.345	1.00	42.90	C
ATOM	1360	CG	ARG	A	173	12.048	42.970	15.527	1.00	41.21	C
ATOM	1361	CD	ARG	A	173	11.096	43.649	16.488	1.00	49.33	C
ATOM	1362	NE	ARG	A	173	9.880	42.862	16.656	1.00	55.21	N
ATOM	1363	CZ	ARG	A	173	8.669	43.387	16.790	1.00	54.70	C
ATOM	1364	NH1	ARG	A	173	8.518	44.704	16.773	1.00	54.11	N
ATOM	1365	NH2	ARG	A	173	7.610	42.596	16.935	1.00	54.36	N
ATOM	1366	N	ILE	A	174	15.135	45.245	13.080	1.00	51.94	N
ATOM	1367	CA	ILE	A	174	16.068	46.331	12.821	1.00	48.52	C
ATOM	1368	C	ILE	A	174	15.228	47.591	12.902	1.00	42.65	C
ATOM	1369	O	ILE	A	174	14.485	47.901	11.973	1.00	40.81	O
ATOM	1370	CB	ILE	A	174	16.687	46.193	11.436	1.00	51.33	C
ATOM	1371	CG1	ILE	A	174	17.536	44.921	11.395	1.00	62.03	C
ATOM	1372	CG2	ILE	A	174	17.536	47.417	11.128	1.00	57.79	C
ATOM	1373	CD1	ILE	A	174	18.075	44.586	10.042	1.00	60.04	C
ATOM	1374	N	LEU	A	175	15.348	48.327	14.004	1.00	43.83	N
ATOM	1375	CA	LEU	A	175	14.514	49.513	14.203	1.00	50.67	C
ATOM	1376	C	LEU	A	175	14.502	50.558	13.102	1.00	53.85	C
ATOM	1377	O	LEU	A	175	13.435	51.017	12.694	1.00	54.58	O
ATOM	1378	CB	LEU	A	175	14.853	50.223	15.520	1.00	52.93	C
ATOM	1379	CG	LEU	A	175	14.067	51.544	15.693	1.00	69.90	C
ATOM	1380	CD1	LEU	A	175	12.539	51.287	15.592	1.00	58.23	C
ATOM	1381	CD2	LEU	A	175	14.423	52.195	17.026	1.00	61.03	C
ATOM	1382	N	ALA	A	176	15.681	50.962	12.641	1.00	49.99	N
ATOM	1383	CA	ALA	A	176	15.753	51.981	11.605	1.00	51.23	C
ATOM	1384	C	ALA	A	176	14.902	51.629	10.385	1.00	45.44	C
ATOM	1385	O	ALA	A	176	14.347	52.518	9.739	1.00	57.30	O
ATOM	1386	CB	ALA	A	176	17.211	52.214	11.193	1.00	54.86	C
ATOM	1387	N	ARG	A	177	14.776	50.341	10.074	1.00	50.42	N
ATOM	1388	CA	ARG	A	177	13.987	49.924	8.917	1.00	45.08	C
ATOM	1389	C	ARG	A	177	12.641	49.302	9.269	1.00	48.67	C
ATOM	1390	O	ARG	A	177	11.862	48.974	8.377	1.00	45.39	O
ATOM	1391	CB	ARG	A	177	14.778	48.918	8.081	1.00	57.24	C
ATOM	1392	CG	ARG	A	177	16.084	49.467	7.544	1.00	64.35	C
ATOM	1393	CD	ARG	A	177	16.813	48.460	6.666	1.00	64.31	C
ATOM	1394	NE	ARG	A	177	17.880	49.138	5.939	1.00	77.29	N
ATOM	1395	CZ	ARG	A	177	17.889	49.331	4.625	1.00	58.44	C
ATOM	1396	NH1	ARG	A	177	16.892	48.883	3.873	1.00	54.23	N
ATOM	1397	NH2	ARG	A	177	18.884	50.009	4.074	1.00	72.33	N
ATOM	1398	N	GLY	A	178	12.373	49.130	10.562	1.00	44.96	N
ATOM	1399	CA	GLY	A	178	11.122	48.508	10.972	1.00	44.41	C
ATOM	1400	C	GLY	A	178	11.050	47.122	10.354	1.00	44.68	C
ATOM	1401	O	GLY	A	178	9.976	46.574	10.092	1.00	40.98	O
ATOM	1402	N	GLU	A	179	12.227	46.544	10.146	1.00	41.13	N
ATOM	1403	CA	GLU	A	179	12.363	45.240	9.513	1.00	46.62	C
ATOM	1404	C	GLU	A	179	12.204	44.076	10.496	1.00	46.51	C
ATOM	1405	O	GLU	A	179	12.710	44.116	11.619	1.00	46.07	O
ATOM	1406	CB	GLU	A	179	13.736	45.192	8.817	1.00	47.47	C
ATOM	1407	CG	GLU	A	179	14.011	44.049	7.852	1.00	52.61	C
ATOM	1408	CD	GLU	A	179	15.396	44.199	7.186	1.00	67.97	C
ATOM	1409	OE1	GLU	A	179	16.232	44.974	7.709	1.00	52.50	O

Figure 2 (Table 2 (page 33))

ATOM	1410	OE2	GLU	A	179	15.657	43.540	6.156	1.00	61.67	O
ATOM	1411	N	ILE	A	180	11.504	43.037	10.044	1.00	46.98	N
ATOM	1412	CA	ILE	A	180	11.260	41.843	10.844	1.00	44.57	C
ATOM	1413	C	ILE	A	180	11.442	40.596	10.028	1.00	49.88	C
ATOM	1414	O	ILE	A	180	11.018	40.531	8.878	1.00	50.41	O
ATOM	1415	CB	ILE	A	180	9.820	41.784	11.371	1.00	60.91	C
ATOM	1416	CG1	ILE	A	180	9.586	42.889	12.387	1.00	56.28	C
ATOM	1417	CG2	ILE	A	180	9.544	40.416	11.996	1.00	58.36	C
ATOM	1418	CD1	ILE	A	180	8.206	42.834	12.973	1.00	63.77	C
ATOM	1419	N	ASN	A	181	12.088	39.607	10.632	1.00	49.49	N
ATOM	1420	CA	ASN	A	181	12.269	38.308	10.010	1.00	44.31	C
ATOM	1421	C	ASN	A	181	12.329	37.382	11.223	1.00	53.84	C
ATOM	1422	O	ASN	A	181	12.789	37.776	12.297	1.00	49.42	O
ATOM	1423	CB	ASN	A	181	13.555	38.240	9.189	1.00	50.86	C
ATOM	1424	CG	ASN	A	181	13.527	37.117	8.165	1.00	58.63	C
ATOM	1425	OD1	ASN	A	181	12.581	36.332	8.126	1.00	68.55	O
ATOM	1426	ND2	ASN	A	181	14.567	37.031	7.331	1.00	62.99	N
ATOM	1427	N	PHE	A	182	11.818	36.172	11.082	1.00	51.66	N
ATOM	1428	CA	PHE	A	182	11.839	35.261	12.210	1.00	54.82	C
ATOM	1429	C	PHE	A	182	12.052	33.843	11.711	1.00	62.75	C
ATOM	1430	O	PHE	A	182	11.914	33.563	10.512	1.00	55.35	O
ATOM	1431	CB	PHE	A	182	10.521	35.354	12.989	1.00	62.28	C
ATOM	1432	CG	PHE	A	182	9.352	34.717	12.283	1.00	74.94	C
ATOM	1433	CD1	PHE	A	182	9.292	33.333	12.120	1.00	82.11	C
ATOM	1434	CD2	PHE	A	182	8.333	35.496	11.745	1.00	81.28	C
ATOM	1435	CE1	PHE	A	182	8.244	32.733	11.429	1.00	84.02	C
ATOM	1436	CE2	PHE	A	182	7.276	34.901	11.049	1.00	84.09	C
ATOM	1437	CZ	PHE	A	182	7.236	33.516	10.892	1.00	83.03	C
ATOM	1438	N	LYS	A	183	12.388	32.946	12.633	1.00	58.39	N
ATOM	1439	CA	LYS	A	183	12.591	31.541	12.295	1.00	50.63	C
ATOM	1440	C	LYS	A	183	12.106	30.678	13.459	1.00	53.23	C
ATOM	1441	O	LYS	A	183	12.431	30.947	14.622	1.00	45.57	O
ATOM	1442	CB	LYS	A	183	14.073	31.263	12.022	1.00	65.15	C
ATOM	1443	CG	LYS	A	183	14.446	29.780	11.957	1.00	64.65	C
ATOM	1444	CD	LYS	A	183	14.295	29.166	10.566	1.00	63.11	C
ATOM	1445	CE	LYS	A	183	14.627	27.670	10.590	1.00	53.42	C
ATOM	1446	NZ	LYS	A	183	15.665	27.264	9.599	1.00	53.61	N
ATOM	1447	N	ASP	A	184	11.319	29.655	13.142	1.00	48.66	N
ATOM	1448	CA	ASP	A	184	10.797	28.751	14.156	1.00	52.92	C
ATOM	1449	C	ASP	A	184	11.722	27.567	14.333	1.00	45.71	C
ATOM	1450	O	ASP	A	184	12.104	26.894	13.371	1.00	44.54	O
ATOM	1451	CB	ASP	A	184	9.404	28.255	13.784	1.00	62.54	C
ATOM	1452	CG	ASP	A	184	8.338	29.306	14.007	1.00	62.50	C
ATOM	1453	OD1	ASP	A	184	8.407	30.010	15.038	1.00	56.56	O
ATOM	1454	OD2	ASP	A	184	7.429	29.417	13.155	1.00	70.30	O
ATOM	1455	N	ILE	A	185	12.085	27.313	15.576	1.00	40.93	N
ATOM	1456	CA	ILE	A	185	12.993	26.219	15.849	1.00	39.71	C
ATOM	1457	C	ILE	A	185	12.372	25.231	16.806	1.00	38.52	C
ATOM	1458	O	ILE	A	185	11.958	25.590	17.909	1.00	38.65	O
ATOM	1459	CB	ILE	A	185	14.326	26.752	16.417	1.00	41.45	C
ATOM	1460	CG1	ILE	A	185	15.051	27.548	15.316	1.00	46.89	C
ATOM	1461	CG2	ILE	A	185	15.199	25.580	16.922	1.00	37.86	C
ATOM	1462	CD1	ILE	A	185	16.246	28.337	15.805	1.00	48.29	C
ATOM	1463	N	GLN	A	186	12.291	23.984	16.355	1.00	42.25	N
ATOM	1464	CA	GLN	A	186	11.744	22.916	17.181	1.00	41.47	C
ATOM	1465	C	GLN	A	186	12.857	22.416	18.097	1.00	38.63	C

Figure 2 (Table 2 (page 34))

ATOM	1466	O	GLN	A	186	13.916	21.991	17.630	1.00	42.48	O
ATOM	1467	CB	GLN	A	186	11.247	21.755	16.307	1.00	52.01	C
ATOM	1468	CG	GLN	A	186	10.732	20.542	17.100	1.00	64.38	C
ATOM	1469	CD	GLN	A	186	10.353	19.348	16.204	1.00	79.51	C
ATOM	1470	OE1	GLN	A	186	10.873	19.202	15.092	1.00	79.17	O
ATOM	1471	NE2	GLN	A	186	9.465	18.481	16.701	1.00	80.31	N
ATOM	1472	N	VAL	A	187	12.610	22.457	19.398	1.00	43.44	N
ATOM	1473	CA	VAL	A	187	13.586	21.987	20.367	1.00	47.67	C
ATOM	1474	C	VAL	A	187	13.146	20.607	20.866	1.00	49.13	C
ATOM	1475	O	VAL	A	187	12.015	20.446	21.311	1.00	40.93	O
ATOM	1476	CB	VAL	A	187	13.675	22.939	21.583	1.00	42.03	C
ATOM	1477	CG1	VAL	A	187	14.563	22.315	22.652	1.00	41.16	C
ATOM	1478	CG2	VAL	A	187	14.224	24.300	21.154	1.00	38.03	C
ATOM	1479	N	ILE	A	188	14.035	19.621	20.785	1.00	41.32	N
ATOM	1480	CA	ILE	A	188	13.733	18.273	21.255	1.00	42.62	C
ATOM	1481	C	ILE	A	188	14.635	17.913	22.441	1.00	40.36	C
ATOM	1482	O	ILE	A	188	15.835	18.224	22.442	1.00	42.29	O
ATOM	1483	CB	ILE	A	188	13.945	17.213	20.142	1.00	45.03	C
ATOM	1484	CG1	ILE	A	188	13.002	17.475	18.967	1.00	41.79	C
ATOM	1485	CG2	ILE	A	188	13.687	15.806	20.702	1.00	46.59	C
ATOM	1486	CD1	ILE	A	188	13.267	16.566	17.763	1.00	40.92	C
ATOM	1487	N	VAL	A	189	14.050	17.285	23.455	1.00	36.36	N
ATOM	1488	CA	VAL	A	189	14.808	16.867	24.627	1.00	42.50	C
ATOM	1489	C	VAL	A	189	14.802	15.338	24.667	1.00	48.22	C
ATOM	1490	O	VAL	A	189	13.748	14.705	24.672	1.00	41.17	O
ATOM	1491	CB	VAL	A	189	14.206	17.455	25.921	1.00	44.30	C
ATOM	1492	CG1	VAL	A	189	14.945	16.930	27.125	1.00	39.49	C
ATOM	1493	CG2	VAL	A	189	14.304	18.966	25.894	1.00	40.56	C
ATOM	1494	N	ASN	A	190	15.993	14.754	24.665	1.00	40.63	N
ATOM	1495	CA	ASN	A	190	16.143	13.316	24.698	1.00	40.98	C
ATOM	1496	C	ASN	A	190	16.395	12.885	26.148	1.00	45.73	C
ATOM	1497	O	ASN	A	190	17.018	13.613	26.918	1.00	45.44	O
ATOM	1498	CB	ASN	A	190	17.285	12.908	23.752	1.00	40.78	C
ATOM	1499	CG	ASN	A	190	16.999	13.293	22.310	1.00	48.31	C
ATOM	1500	OD1	ASN	A	190	15.917	13.005	21.782	1.00	44.75	O
ATOM	1501	ND2	ASN	A	190	17.962	13.951	21.664	1.00	41.66	N
ATOM	1502	N	VAL	A	191	15.877	11.710	26.509	1.00	42.84	N
ATOM	1503	CA	VAL	A	191	15.982	11.151	27.863	1.00	39.39	C
ATOM	1504	C	VAL	A	191	16.683	9.802	27.788	1.00	39.64	C
ATOM	1505	O	VAL	A	191	16.261	8.910	27.043	1.00	47.40	O
ATOM	1506	CB	VAL	A	191	14.574	10.954	28.470	1.00	44.63	C
ATOM	1507	CG1	VAL	A	191	14.671	10.368	29.890	1.00	41.78	C
ATOM	1508	CG2	VAL	A	191	13.848	12.310	28.499	1.00	41.72	C
ATOM	1509	N	PRO	A	192	17.775	9.641	28.542	1.00	43.27	N
ATOM	1510	CA	PRO	A	192	18.578	8.416	28.596	1.00	45.21	C
ATOM	1511	C	PRO	A	192	17.722	7.224	28.990	1.00	42.00	C
ATOM	1512	O	PRO	A	192	16.783	7.355	29.763	1.00	42.35	O
ATOM	1513	CB	PRO	A	192	19.620	8.737	29.668	1.00	49.92	C
ATOM	1514	CG	PRO	A	192	19.690	10.204	29.687	1.00	49.81	C
ATOM	1515	CD	PRO	A	192	18.246	10.602	29.556	1.00	43.30	C
ATOM	1516	N	PRO	A	193	18.075	6.034	28.515	1.00	40.57	N
ATOM	1517	CA	PRO	A	193	17.301	4.848	28.838	1.00	39.79	C
ATOM	1518	C	PRO	A	193	17.516	4.372	30.256	1.00	43.45	C
ATOM	1519	O	PRO	A	193	18.552	4.666	30.864	1.00	44.20	O
ATOM	1520	CB	PRO	A	193	17.842	3.809	27.853	1.00	41.07	C
ATOM	1521	CG	PRO	A	193	18.661	4.630	26.843	1.00	46.01	C

Figure 2 (Table 2 (page 35))

ATOM	1522	CD	PRO	A	193	19.250	5.657	27.729	1.00	47.13	C
ATOM	1523	N	THR	A	194	16.516	3.665	30.779	1.00	45.04	N
ATOM	1524	CA	THR	A	194	16.614	2.987	32.075	1.00	48.33	C
ATOM	1525	C	THR	A	194	16.019	1.623	31.713	1.00	51.40	C
ATOM	1526	O	THR	A	194	15.124	1.529	30.848	1.00	41.84	O
ATOM	1527	CB	THR	A	194	15.792	3.630	33.225	1.00	48.61	C
ATOM	1528	OG1	THR	A	194	14.414	3.724	32.862	1.00	54.30	O
ATOM	1529	CG2	THR	A	194	16.338	4.992	33.574	1.00	57.24	C
ATOM	1530	N	VAL	A	195	16.507	0.565	32.352	1.00	48.50	N
ATOM	1531	CA	VAL	A	195	16.026	-0.760	32.017	1.00	45.60	C
ATOM	1532	C	VAL	A	195	16.083	-1.715	33.200	1.00	42.61	C
ATOM	1533	O	VAL	A	195	16.976	-1.644	34.021	1.00	46.25	O
ATOM	1534	CB	VAL	A	195	16.853	-1.346	30.840	1.00	42.93	C
ATOM	1535	CG1	VAL	A	195	18.314	-1.582	31.282	1.00	43.08	C
ATOM	1536	CG2	VAL	A	195	16.218	-2.635	30.339	1.00	43.46	C
ATOM	1537	N	GLN	A	196	15.104	-2.603	33.282	1.00	41.51	N
ATOM	1538	CA	GLN	A	196	15.070	-3.577	34.355	1.00	48.63	C
ATOM	1539	C	GLN	A	196	14.615	-4.928	33.817	1.00	46.66	C
ATOM	1540	O	GLN	A	196	13.706	-5.009	32.992	1.00	45.71	O
ATOM	1541	CB	GLN	A	196	14.119	-3.118	35.477	1.00	49.59	C
ATOM	1542	CG	GLN	A	196	14.693	-2.064	36.393	1.00	55.69	C
ATOM	1543	CD	GLN	A	196	13.790	-1.757	37.588	1.00	74.35	C
ATOM	1544	OE1	GLN	A	196	14.268	-1.328	38.639	1.00	74.51	O
ATOM	1545	NE2	GLN	A	196	12.482	-1.970	37.429	1.00	79.78	N
ATOM	1546	N	ALA	A	197	15.257	-5.991	34.282	1.00	40.70	N
ATOM	1547	CA	ALA	A	197	14.876	-7.329	33.873	1.00	39.75	C
ATOM	1548	C	ALA	A	197	13.550	-7.650	34.550	1.00	42.61	C
ATOM	1549	O	ALA	A	197	13.316	-7.246	35.687	1.00	48.54	O
ATOM	1550	CB	ALA	A	197	15.940	-8.333	34.313	1.00	39.72	C
ATOM	1551	N	ARG	A	198	12.671	-8.368	33.865	1.00	43.54	N
ATOM	1552	CA	ARG	A	198	11.403	-8.720	34.485	1.00	44.25	C
ATOM	1553	C	ARG	A	198	11.664	-9.866	35.479	1.00	53.02	C
ATOM	1554	O	ARG	A	198	11.018	-9.960	36.528	1.00	45.60	O
ATOM	1555	CB	ARG	A	198	10.392	-9.131	33.416	1.00	49.38	C
ATOM	1556	CG	ARG	A	198	8.967	-8.992	33.873	1.00	56.08	C
ATOM	1557	CD	ARG	A	198	7.991	-9.099	32.724	1.00	58.30	C
ATOM	1558	NE	ARG	A	198	7.873	-7.869	31.947	1.00	47.20	N
ATOM	1559	CZ	ARG	A	198	6.931	-7.675	31.030	1.00	54.23	C
ATOM	1560	NH1	ARG	A	198	6.038	-8.633	30.793	1.00	47.47	N
ATOM	1561	NH2	ARG	A	198	6.882	-6.541	30.339	1.00	50.85	N
ATOM	1562	N	GLN	A	199	12.625	-10.722	35.133	1.00	51.86	N
ATOM	1563	CA	GLN	A	199	13.047	-11.844	35.965	1.00	52.79	C
ATOM	1564	C	GLN	A	199	14.564	-11.926	35.871	1.00	50.17	C
ATOM	1565	O	GLN	A	199	15.107	-12.162	34.798	1.00	54.53	O
ATOM	1566	CB	GLN	A	199	12.447	-13.159	35.472	1.00	58.34	C
ATOM	1567	CG	GLN	A	199	10.941	-13.292	35.635	1.00	68.50	C
ATOM	1568	CD	GLN	A	199	10.498	-13.315	37.100	1.00	83.24	C
ATOM	1569	OE1	GLN	A	199	11.300	-13.596	37.996	1.00	85.74	O
ATOM	1570	NE2	GLN	A	199	9.214	-13.035	37.347	1.00	71.40	N
ATOM	1571	N	SER	A	200	15.247	-11.719	36.991	1.00	46.12	N
ATOM	1572	CA	SER	A	200	16.715	-11.753	37.042	1.00	50.15	C
ATOM	1573	C	SER	A	200	17.328	-13.157	37.004	1.00	47.60	C
ATOM	1574	O	SER	A	200	18.458	-13.350	36.541	1.00	49.49	O
ATOM	1575	CB	SER	A	200	17.194	-11.061	38.318	1.00	49.46	C
ATOM	1576	OG	SER	A	200	16.702	-9.737	38.384	1.00	76.11	O
ATOM	1577	N	ILE	A	201	16.576	-14.122	37.518	1.00	48.87	N

Figure 2 (Table 2 (page 36))

ATOM	1578	CA	ILE	A	201	17.019	-15.504	37.591	1.00 50.62	C
ATOM	1579	C	ILE	A	201	15.994	-16.400	36.925	1.00 47.35	C
ATOM	1580	O	ILE	A	201	14.797	-16.328	37.216	1.00 51.41	O
ATOM	1581	CB	ILE	A	201	17.181	-15.962	39.067	1.00 64.29	C
ATOM	1582	CG1	ILE	A	201	18.080	-14.983	39.838	1.00 57.76	C
ATOM	1583	CG2	ILE	A	201	17.768	-17.373	39.116	1.00 58.42	C
ATOM	1584	CD1	ILE	A	201	19.476	-14.860	39.290	1.00 68.87	C
ATOM	1585	N	VAL	A	202	16.469	-17.249	36.032	1.00 46.21	N
ATOM	1586	CA	VAL	A	202	15.587	-18.157	35.339	1.00 49.25	C
ATOM	1587	C	VAL	A	202	16.207	-19.540	35.336	1.00 47.17	C
ATOM	1588	O	VAL	A	202	17.391	-19.687	35.045	1.00 43.79	O
ATOM	1589	CB	VAL	A	202	15.371	-17.701	33.882	1.00 53.12	C
ATOM	1590	CG1	VAL	A	202	14.436	-18.661	33.177	1.00 45.19	C
ATOM	1591	CG2	VAL	A	202	14.820	-16.276	33.861	1.00 50.64	C
ATOM	1592	N	ASN	A	203	15.393	-20.544	35.653	1.00 49.57	N
ATOM	1593	CA	ASN	A	203	15.827	-21.937	35.680	1.00 51.28	C
ATOM	1594	C	ASN	A	203	15.078	-22.676	34.575	1.00 55.81	C
ATOM	1595	O	ASN	A	203	13.857	-22.541	34.440	1.00 50.57	O
ATOM	1596	CB	ASN	A	203	15.473	-22.635	37.010	1.00 49.03	C
ATOM	1597	CG	ASN	A	203	16.218	-22.067	38.217	1.00 47.83	C
ATOM	1598	OD1	ASN	A	203	17.319	-21.530	38.105	1.00 47.54	O
ATOM	1599	ND2	ASN	A	203	15.617	-22.217	39.390	1.00 44.22	N
ATOM	1600	N	ALA	A	204	15.811	-23.487	33.825	1.00 53.79	N
ATOM	1601	CA	ALA	A	204	15.249	-24.272	32.738	1.00 58.78	C
ATOM	1602	C	ALA	A	204	15.827	-25.683	32.730	1.00 59.86	C
ATOM	1603	O	ALA	A	204	16.909	-25.933	33.268	1.00 58.63	O
ATOM	1604	CB	ALA	A	204	15.541	-23.592	31.408	1.00 54.08	C
ATOM	1605	N	THR	A	205	15.088	-26.592	32.100	1.00 63.01	N
ATOM	1606	CA	THR	A	205	15.483	-27.989	31.966	1.00 62.26	C
ATOM	1607	C	THR	A	205	15.949	-28.248	30.546	1.00 59.60	C
ATOM	1608	O	THR	A	205	15.282	-27.874	29.579	1.00 57.70	O
ATOM	1609	CB	THR	A	205	14.323	-28.946	32.265	1.00 63.31	C
ATOM	1610	OG1	THR	A	205	13.916	-28.799	33.634	1.00 64.86	O
ATOM	1611	CG2	THR	A	205	14.760	-30.383	32.012	1.00 70.94	C
ATOM	1612	N	ALA	A	206	17.089	-28.913	30.430	1.00 56.34	N
ATOM	1613	CA	ALA	A	206	17.670	-29.203	29.134	1.00 60.33	C
ATOM	1614	C	ALA	A	206	17.035	-30.352	28.375	1.00 64.54	C
ATOM	1615	O	ALA	A	206	16.377	-31.228	28.940	1.00 68.98	O
ATOM	1616	CB	ALA	A	206	19.156	-29.464	29.290	1.00 58.07	C
ATOM	1617	N	ASN	A	207	17.246	-30.306	27.067	1.00 71.10	N
ATOM	1618	CA	ASN	A	207	16.791	-31.322	26.140	1.00 71.82	C
ATOM	1619	C	ASN	A	207	15.352	-31.788	26.216	1.00 70.92	C
ATOM	1620	O	ASN	A	207	15.077	-32.971	26.023	1.00 73.91	O
ATOM	1621	CB	ASN	A	207	17.724	-32.518	26.249	1.00 69.97	C
ATOM	1622	CG	ASN	A	207	19.170	-32.119	26.105	1.00 75.29	C
ATOM	1623	OD1	ASN	A	207	19.562	-31.531	25.097	1.00 81.94	O
ATOM	1624	ND2	ASN	A	207	19.972	-32.421	27.115	1.00 80.72	N
ATOM	1625	N	LEU	A	208	14.432	-30.877	26.496	1.00 67.07	N
ATOM	1626	CA	LEU	A	208	13.026	-31.246	26.528	1.00 68.52	C
ATOM	1627	C	LEU	A	208	12.347	-30.484	25.391	1.00 67.74	C
ATOM	1628	O	LEU	A	208	11.122	-30.415	25.306	1.00 73.14	O
ATOM	1629	CB	LEU	A	208	12.393	-30.904	27.877	1.00 68.09	C
ATOM	1630	CG	LEU	A	208	12.930	-31.679	29.091	1.00 79.90	C
ATOM	1631	CD1	LEU	A	208	12.105	-31.321	30.319	1.00 73.01	C
ATOM	1632	CD2	LEU	A	208	12.854	-33.180	28.843	1.00 77.54	C
ATOM	1633	N	GLY	A	209	13.175	-29.907	24.519	1.00 74.00	N

Figure 2 (Table 2 (page 37))

ATOM	1634	CA	GLY	A	209	12.694	-29.159	23.364	1.00	81.72	C
ATOM	1635	C	GLY	A	209	11.907	-27.893	23.667	1.00	87.49	C
ATOM	1636	O	GLY	A	209	11.241	-27.341	22.788	1.00	95.12	O
ATOM	1637	N	GLN	A	210	11.992	-27.420	24.905	1.00	84.00	N
ATOM	1638	CA	GLN	A	210	11.254	-26.230	25.299	1.00	82.13	C
ATOM	1639	C	GLN	A	210	12.033	-24.922	25.205	1.00	74.00	C
ATOM	1640	O	GLN	A	210	13.265	-24.922	25.132	1.00	71.75	O
ATOM	1641	CB	GLN	A	210	10.703	-26.400	26.711	1.00	86.64	C
ATOM	1642	CG	GLN	A	210	11.770	-26.685	27.754	1.00	92.84	C
ATOM	1643	CD	GLN	A	210	11.215	-27.469	28.932	1.00	98.28	C
ATOM	1644	OE1	GLN	A	210	10.047	-27.856	28.930	1.00	102.57	O
ATOM	1645	NE2	GLN	A	210	12.049	-27.714	29.938	1.00	100.49	N
ATOM	1646	N	SER	A	211	11.295	-23.810	25.212	1.00	73.42	N
ATOM	1647	CA	SER	A	211	11.873	-22.470	25.101	1.00	68.89	C
ATOM	1648	C	SER	A	211	11.749	-21.688	26.394	1.00	59.63	C
ATOM	1649	O	SER	A	211	10.995	-22.044	27.297	1.00	58.00	O
ATOM	1650	CB	SER	A	211	11.181	-21.680	23.978	1.00	69.06	C
ATOM	1651	OG	SER	A	211	11.312	-22.319	22.719	1.00	75.29	O
ATOM	1652	N	VAL	A	212	12.515	-20.616	26.479	1.00	62.83	N
ATOM	1653	CA	VAL	A	212	12.470	-19.749	27.638	1.00	57.69	C
ATOM	1654	C	VAL	A	212	12.482	-18.343	27.056	1.00	51.71	C
ATOM	1655	O	VAL	A	212	13.140	-18.086	26.044	1.00	48.36	O
ATOM	1656	CB	VAL	A	212	13.697	-19.965	28.554	1.00	58.76	C
ATOM	1657	CG1	VAL	A	212	14.970	-19.802	27.762	1.00	57.99	C
ATOM	1658	CG2	VAL	A	212	13.665	-18.988	29.707	1.00	65.40	C
ATOM	1659	N	THR	A	213	11.738	-17.438	27.672	1.00	48.53	N
ATOM	1660	CA	THR	A	213	11.698	-16.079	27.171	1.00	50.94	C
ATOM	1661	C	THR	A	213	12.279	-15.100	28.194	1.00	46.89	C
ATOM	1662	O	THR	A	213	11.760	-14.969	29.301	1.00	48.85	O
ATOM	1663	CB	THR	A	213	10.246	-15.669	26.820	1.00	50.59	C
ATOM	1664	OG1	THR	A	213	9.720	-16.556	25.827	1.00	54.06	O
ATOM	1665	CG2	THR	A	213	10.214	-14.255	26.276	1.00	56.06	C
ATOM	1666	N	LEU	A	214	13.367	-14.430	27.823	1.00	50.67	N
ATOM	1667	CA	LEU	A	214	14.015	-13.445	28.686	1.00	44.75	C
ATOM	1668	C	LEU	A	214	13.444	-12.078	28.327	1.00	49.46	C
ATOM	1669	O	LEU	A	214	13.339	-11.738	27.147	1.00	40.16	O
ATOM	1670	CB	LEU	A	214	15.519	-13.469	28.464	1.00	40.05	C
ATOM	1671	CG	LEU	A	214	16.140	-14.857	28.611	1.00	47.06	C
ATOM	1672	CD1	LEU	A	214	17.647	-14.728	28.666	1.00	41.62	C
ATOM	1673	CD2	LEU	A	214	15.623	-15.532	29.880	1.00	42.47	C
ATOM	1674	N	VAL	A	215	13.089	-11.299	29.345	1.00	44.86	N
ATOM	1675	CA	VAL	A	215	12.454	-10.004	29.143	1.00	46.92	C
ATOM	1676	C	VAL	A	215	13.030	-8.850	29.928	1.00	48.90	C
ATOM	1677	O	VAL	A	215	13.254	-8.937	31.135	1.00	50.91	O
ATOM	1678	CB	VAL	A	215	10.969	-10.089	29.508	1.00	49.64	C
ATOM	1679	CG1	VAL	A	215	10.265	-8.759	29.213	1.00	50.90	C
ATOM	1680	CG2	VAL	A	215	10.332	-11.234	28.765	1.00	52.37	C
ATOM	1681	N	CYS	A	216	13.254	-7.755	29.221	1.00	44.39	N
ATOM	1682	CA	CYS	A	216	13.754	-6.542	29.826	1.00	45.29	C
ATOM	1683	C	CYS	A	216	12.744	-5.449	29.501	1.00	52.26	C
ATOM	1684	O	CYS	A	216	12.223	-5.399	28.393	1.00	47.28	O
ATOM	1685	CB	CYS	A	216	15.122	-6.180	29.257	1.00	45.92	C
ATOM	1686	SG	CYS	A	216	16.483	-7.140	29.998	1.00	51.48	S
ATOM	1687	N	ASP	A	217	12.454	-4.598	30.478	1.00	44.49	N
ATOM	1688	CA	ASP	A	217	11.523	-3.499	30.291	1.00	46.18	C
ATOM	1689	C	ASP	A	217	12.330	-2.230	30.313	1.00	46.02	C

Figure 2 (Table 2 (page 38))

ATOM	1690	O	ASP	A	217	12.974	-1.906	31.307	1.00	42.34	O
ATOM	1691	CB	ASP	A	217	10.501	-3.453	31.419	1.00	43.07	C
ATOM	1692	CG	ASP	A	217	9.576	-4.624	31.382	1.00	54.67	C
ATOM	1693	OD1	ASP	A	217	8.860	-4.755	30.366	1.00	54.44	O
ATOM	1694	OD2	ASP	A	217	9.573	-5.417	32.350	1.00	52.78	O
ATOM	1695	N	ALA	A	218	12.279	-1.498	29.215	1.00	43.43	N
ATOM	1696	CA	ALA	A	218	13.030	-0.269	29.129	1.00	51.56	C
ATOM	1697	C	ALA	A	218	12.205	0.900	28.633	1.00	51.78	C
ATOM	1698	O	ALA	A	218	11.150	0.731	28.031	1.00	48.04	O
ATOM	1699	CB	ALA	A	218	14.221	-0.468	28.202	1.00	46.61	C
ATOM	1700	N	ASP	A	219	12.704	2.096	28.901	1.00	47.98	N
ATOM	1701	CA	ASP	A	219	12.076	3.287	28.377	1.00	53.40	C
ATOM	1702	C	ASP	A	219	13.097	4.412	28.287	1.00	54.39	C
ATOM	1703	O	ASP	A	219	14.214	4.308	28.791	1.00	53.10	O
ATOM	1704	CB	ASP	A	219	10.876	3.693	29.214	1.00	67.27	C
ATOM	1705	CG	ASP	A	219	11.226	3.878	30.644	1.00	73.00	C
ATOM	1706	OD1	ASP	A	219	12.424	4.087	30.905	1.00	77.65	O
ATOM	1707	OD2	ASP	A	219	10.315	3.824	31.502	1.00	83.21	O
ATOM	1708	N	GLY	A	220	12.693	5.482	27.622	1.00	46.12	N
ATOM	1709	CA	GLY	A	220	13.541	6.632	27.405	1.00	43.59	C
ATOM	1710	C	GLY	A	220	13.035	7.286	26.135	1.00	46.49	C
ATOM	1711	O	GLY	A	220	12.062	6.810	25.554	1.00	45.48	O
ATOM	1712	N	PHE	A	221	13.700	8.341	25.678	1.00	43.50	N
ATOM	1713	CA	PHE	A	221	13.283	9.017	24.465	1.00	42.29	C
ATOM	1714	C	PHE	A	221	14.499	9.499	23.669	1.00	33.90	C
ATOM	1715	O	PHE	A	221	15.313	10.265	24.178	1.00	43.58	O
ATOM	1716	CB	PHE	A	221	12.391	10.215	24.797	1.00	41.04	C
ATOM	1717	CG	PHE	A	221	11.792	10.861	23.572	1.00	44.52	C
ATOM	1718	CD1	PHE	A	221	10.591	10.395	23.037	1.00	47.33	C
ATOM	1719	CD2	PHE	A	221	12.482	11.863	22.891	1.00	44.34	C
ATOM	1720	CE1	PHE	A	221	10.088	10.910	21.837	1.00	45.26	C
ATOM	1721	CE2	PHE	A	221	11.989	12.380	21.693	1.00	48.97	C
ATOM	1722	CZ	PHE	A	221	10.785	11.897	21.166	1.00	44.61	C
ATOM	1723	N	PRO	A	222	14.645	9.050	22.400	1.00	40.11	N
ATOM	1724	CA	PRO	A	222	13.780	8.122	21.655	1.00	40.06	C
ATOM	1725	C	PRO	A	222	13.693	6.765	22.344	1.00	50.45	C
ATOM	1726	O	PRO	A	222	14.546	6.419	23.172	1.00	43.37	O
ATOM	1727	CB	PRO	A	222	14.480	8.000	20.307	1.00	44.90	C
ATOM	1728	CG	PRO	A	222	15.163	9.311	20.158	1.00	43.89	C
ATOM	1729	CD	PRO	A	222	15.733	9.547	21.536	1.00	38.16	C
ATOM	1730	N	GLU	A	223	12.659	5.999	21.998	1.00	47.32	N
ATOM	1731	CA	GLU	A	223	12.466	4.664	22.565	1.00	48.48	C
ATOM	1732	C	GLU	A	223	13.778	3.917	22.403	1.00	44.89	C
ATOM	1733	O	GLU	A	223	14.364	3.886	21.321	1.00	42.04	O
ATOM	1734	CB	GLU	A	223	11.359	3.905	21.837	1.00	51.24	C
ATOM	1735	CG	GLU	A	223	9.947	4.402	22.100	1.00	45.06	C
ATOM	1736	CD	GLU	A	223	9.513	4.303	23.556	1.00	60.54	C
ATOM	1737	OE1	GLU	A	223	9.950	3.368	24.263	1.00	71.83	O
ATOM	1738	OE2	GLU	A	223	8.700	5.153	23.986	1.00	70.97	O
ATOM	1739	N	PRO	A	224	14.249	3.296	23.483	1.00	46.34	N
ATOM	1740	CA	PRO	A	224	15.507	2.559	23.453	1.00	48.92	C
ATOM	1741	C	PRO	A	224	15.536	1.373	22.501	1.00	49.30	C
ATOM	1742	O	PRO	A	224	14.535	0.692	22.311	1.00	47.42	O
ATOM	1743	CB	PRO	A	224	15.678	2.113	24.911	1.00	47.68	C
ATOM	1744	CG	PRO	A	224	14.893	3.128	25.698	1.00	57.81	C
ATOM	1745	CD	PRO	A	224	13.673	3.314	24.843	1.00	47.48	C

Figure 2 (Table 2 (page 39))

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ATOM   1746  N    THR A 225     16.685    1.143   21.884  1.00  50.13  N
ATOM   1747  CA   THR A 225     16.859   -0.016   21.021  1.00  60.61  C
ATOM   1748  C    THR A 225     17.598   -1.033   21.907  1.00  59.15  C
ATOM   1749  O    THR A 225     18.533   -0.663   22.631  1.00  47.10  O
ATOM   1750  CB   THR A 225     17.723    0.319   19.810  1.00  58.08  C
ATOM   1751  OG1  THR A 225     17.027    1.259   18.985  1.00  83.82  O
ATOM   1752  CG2  THR A 225     18.009   -0.934   19.003  1.00  73.24  C
ATOM   1753  N    MET A 226     17.189   -2.296   21.862  1.00  52.21  N
ATOM   1754  CA   MET A 226     17.824   -3.310   22.692  1.00  53.46  C
ATOM   1755  C    MET A 226     18.721   -4.265   21.927  1.00  56.38  C
ATOM   1756  O    MET A 226     18.417   -4.657   20.802  1.00  51.69  O
ATOM   1757  CB   MET A 226     16.766   -4.149   23.397  1.00  61.02  C
ATOM   1758  CG   MET A 226     15.711   -3.339   24.112  1.00  73.13  C
ATOM   1759  SD   MET A 226     16.515   -2.409   25.388  1.00  79.72  S
ATOM   1760  CE   MET A 226     17.052   -3.791   26.474  1.00  72.80  C
ATOM   1761  N    SER A 227     19.821   -4.649   22.564  1.00  51.74  N
ATOM   1762  CA   SER A 227     20.755   -5.617   22.003  1.00  57.86  C
ATOM   1763  C    SER A 227     21.169   -6.496   23.187  1.00  61.93  C
ATOM   1764  O    SER A 227     21.204   -6.024   24.332  1.00  60.05  O
ATOM   1765  CB   SER A 227     21.961   -4.912   21.403  1.00  41.57  C
ATOM   1766  OG   SER A 227     22.546   -4.056   22.355  1.00  62.88  O
ATOM   1767  N    TRP A 228     21.472   -7.765   22.924  1.00  57.15  N
ATOM   1768  CA   TRP A 228     21.840   -8.689   23.998  1.00  55.47  C
ATOM   1769  C    TRP A 228     23.243   -9.290   23.899  1.00  59.04  C
ATOM   1770  O    TRP A 228     23.856   -9.273   22.829  1.00  49.40  O
ATOM   1771  CB   TRP A 228     20.842   -9.840   24.050  1.00  49.35  C
ATOM   1772  CG   TRP A 228     19.435   -9.439   24.308  1.00  47.96  C
ATOM   1773  CD1  TRP A 228     18.630   -8.695   23.494  1.00  53.38  C
ATOM   1774  CD2  TRP A 228     18.654   -9.760   25.462  1.00  47.76  C
ATOM   1775  NE1  TRP A 228     17.394   -8.537   24.067  1.00  52.08  N
ATOM   1776  CE2  TRP A 228     17.379   -9.177   25.279  1.00  45.77  C
ATOM   1777  CE3  TRP A 228     18.906  -10.482   26.637  1.00  42.71  C
ATOM   1778  CZ2  TRP A 228     16.355   -9.291   26.227  1.00  37.55  C
ATOM   1779  CZ3  TRP A 228     17.887  -10.598   27.586  1.00  45.83  C
ATOM   1780  CH2  TRP A 228     16.625  -10.004   27.373  1.00  50.85  C
ATOM   1781  N    THR A 229     23.749   -9.795   25.027  1.00  58.07  N
ATOM   1782  CA   THR A 229     25.047  -10.474   25.057  1.00  60.10  C
ATOM   1783  C    THR A 229     24.918  -11.741   25.902  1.00  61.83  C
ATOM   1784  O    THR A 229     24.132  -11.787   26.868  1.00  54.86  O
ATOM   1785  CB   THR A 229     26.191   -9.610   25.652  1.00  53.98  C
ATOM   1786  OG1  THR A 229     25.882   -9.252   26.999  1.00  57.01  O
ATOM   1787  CG2  THR A 229     26.418   -8.373   24.816  1.00  57.89  C
ATOM   1788  N    LYS A 230     25.677  -12.765   25.515  1.00  58.82  N
ATOM   1789  CA   LYS A 230     25.684  -14.043   26.217  1.00  58.37  C
ATOM   1790  C    LYS A 230     27.088  -14.147   26.792  1.00  52.83  C
ATOM   1791  O    LYS A 230     28.066  -14.266   26.054  1.00  54.49  O
ATOM   1792  CB   LYS A 230     25.396  -15.173   25.227  1.00  55.01  C
ATOM   1793  CG   LYS A 230     25.113  -16.539   25.849  1.00  45.56  C
ATOM   1794  CD   LYS A 230     24.973  -17.615   24.757  1.00  59.41  C
ATOM   1795  CE   LYS A 230     24.803  -19.019   25.339  1.00  62.34  C
ATOM   1796  NZ   LYS A 230     24.460  -20.050   24.304  1.00  59.23  N
ATOM   1797  N    ASP A 231     27.183  -14.078   28.115  1.00  61.62  N
ATOM   1798  CA   ASP A 231     28.479  -14.105   28.781  1.00  69.33  C
ATOM   1799  C    ASP A 231     29.439  -13.118   28.113  1.00  69.66  C
ATOM   1800  O    ASP A 231     30.612  -13.429   27.916  1.00  73.37  O
ATOM   1801  CB   ASP A 231     29.096  -15.509   28.754  1.00  67.95  C
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Figure 2 (Table 2 (page 40))

ATOM	1802	CG	ASP	A	231	28.359	-16.492	29.645	1.00	76.63	C
ATOM	1803	OD1	ASP	A	231	27.830	-16.069	30.697	1.00	73.37	O
ATOM	1804	OD2	ASP	A	231	28.327	-17.692	29.295	1.00	73.07	O
ATOM	1805	N	GLY	A	232	28.939	-11.933	27.766	1.00	69.81	N
ATOM	1806	CA	GLY	A	232	29.780	-10.925	27.147	1.00	62.92	C
ATOM	1807	C	GLY	A	232	29.815	-10.953	25.633	1.00	57.21	C
ATOM	1808	O	GLY	A	232	30.217	-9.985	24.999	1.00	64.11	O
ATOM	1809	N	GLU	A	233	29.398	-12.058	25.039	1.00	60.24	N
ATOM	1810	CA	GLU	A	233	29.407	-12.163	23.587	1.00	67.77	C
ATOM	1811	C	GLU	A	233	28.086	-11.753	22.977	1.00	69.76	C
ATOM	1812	O	GLU	A	233	27.019	-12.146	23.437	1.00	67.85	O
ATOM	1813	CB	GLU	A	233	29.721	-13.589	23.156	1.00	73.47	C
ATOM	1814	CG	GLU	A	233	31.174	-13.980	23.298	1.00	93.05	C
ATOM	1815	CD	GLU	A	233	32.100	-13.154	22.416	1.00	101.69	C
ATOM	1816	OE1	GLU	A	233	31.753	-12.894	21.241	1.00	104.10	O
ATOM	1817	OE2	GLU	A	233	33.189	-12.771	22.898	1.00	105.15	O
ATOM	1818	N	PRO	A	234	28.146	-10.986	21.894	1.00	69.71	N
ATOM	1819	CA	PRO	A	234	26.928	-10.527	21.227	1.00	69.07	C
ATOM	1820	C	PRO	A	234	26.042	-11.660	20.747	1.00	63.95	C
ATOM	1821	O	PRO	A	234	26.516	-12.774	20.513	1.00	68.33	O
ATOM	1822	CB	PRO	A	234	27.463	-9.717	20.047	1.00	74.23	C
ATOM	1823	CG	PRO	A	234	28.863	-9.346	20.458	1.00	78.24	C
ATOM	1824	CD	PRO	A	234	29.349	-10.575	21.151	1.00	73.22	C
ATOM	1825	N	ILE	A	235	24.756	-11.361	20.589	1.00	60.42	N
ATOM	1826	CA	ILE	A	235	23.819	-12.347	20.075	1.00	59.30	C
ATOM	1827	C	ILE	A	235	23.091	-11.707	18.887	1.00	73.94	C
ATOM	1828	O	ILE	A	235	22.292	-10.780	19.062	1.00	69.18	O
ATOM	1829	CB	ILE	A	235	22.785	-12.748	21.118	1.00	58.75	C
ATOM	1830	CG1	ILE	A	235	23.480	-13.103	22.435	1.00	60.61	C
ATOM	1831	CG2	ILE	A	235	21.986	-13.935	20.602	1.00	54.52	C
ATOM	1832	CD1	ILE	A	235	22.535	-13.237	23.598	1.00	58.31	C
ATOM	1833	N	GLU	A	236	23.341	-12.205	17.679	1.00	80.94	N
ATOM	1834	CA	GLU	A	236	22.742	-11.605	16.488	1.00	90.13	C
ATOM	1835	C	GLU	A	236	21.234	-11.755	16.308	1.00	93.13	C
ATOM	1836	O	GLU	A	236	20.685	-12.857	16.339	1.00	89.58	O
ATOM	1837	CB	GLU	A	236	23.493	-12.094	15.252	1.00	98.19	C
ATOM	1838	CG	GLU	A	236	25.017	-12.039	15.429	1.00	107.77	C
ATOM	1839	CD	GLU	A	236	25.542	-10.662	15.844	1.00	115.02	C
ATOM	1840	OE1	GLU	A	236	24.988	-10.055	16.788	1.00	121.81	O
ATOM	1841	OE2	GLU	A	236	26.526	-10.191	15.233	1.00	116.63	O
ATOM	1842	N	ASN	A	237	20.585	-10.606	16.115	1.00	98.73	N
ATOM	1843	CA	ASN	A	237	19.136	-10.494	15.944	1.00	104.56	C
ATOM	1844	C	ASN	A	237	18.609	-11.196	14.686	1.00	110.81	C
ATOM	1845	O	ASN	A	237	17.530	-11.792	14.705	1.00	112.81	O
ATOM	1846	CB	ASN	A	237	18.759	-9.004	15.930	1.00	100.46	C
ATOM	1847	CG	ASN	A	237	17.268	-8.761	16.142	1.00	100.48	C
ATOM	1848	OD1	ASN	A	237	16.868	-7.689	16.600	1.00	96.36	O
ATOM	1849	ND2	ASN	A	237	16.443	-9.747	15.798	1.00	97.08	N
ATOM	1850	N	GLU	A	238	19.382	-11.111	13.607	1.00	114.86	N
ATOM	1851	CA	GLU	A	238	19.072	-11.709	12.303	1.00	120.04	C
ATOM	1852	C	GLU	A	238	17.688	-12.328	12.095	1.00	121.21	C
ATOM	1853	O	GLU	A	238	16.975	-11.855	11.181	1.00	121.72	O
ATOM	1854	CB	GLU	A	238	20.152	-12.736	11.963	1.00	121.17	C
ATOM	1855	CG	GLU	A	238	21.557	-12.228	12.238	1.00	126.14	C
ATOM	1856	CD	GLU	A	238	21.808	-10.840	11.662	1.00	130.48	C
ATOM	1857	OE1	GLU	A	238	21.090	-9.885	12.034	1.00	132.56	O

Figure 2 (Table 2 (page 41))

ATOM	1858	OE2	GLU	A	238	22.731	-10.705	10.837	1.00	134.55	O
ATOM	1859	N	ASP	A	241	18.070	-14.713	9.305	1.00	127.03	N
ATOM	1860	CA	ASP	A	241	17.685	-16.080	9.767	1.00	127.98	C
ATOM	1861	C	ASP	A	241	17.960	-16.274	11.255	1.00	129.18	C
ATOM	1862	O	ASP	A	241	18.938	-15.754	11.803	1.00	129.01	O
ATOM	1863	CB	ASP	A	241	18.443	-17.152	8.972	1.00	124.42	C
ATOM	1864	CG	ASP	A	241	18.044	-18.574	9.365	1.00	123.20	C
ATOM	1865	OD1	ASP	A	241	18.114	-18.916	10.570	1.00	119.17	O
ATOM	1866	OD2	ASP	A	241	17.664	-19.356	8.464	1.00	120.27	O
ATOM	1867	N	ASP	A	242	17.080	-17.043	11.888	1.00	129.87	N
ATOM	1868	CA	ASP	A	242	17.157	-17.357	13.310	1.00	128.52	C
ATOM	1869	C	ASP	A	242	16.420	-18.676	13.544	1.00	124.12	C
ATOM	1870	O	ASP	A	242	15.291	-18.851	13.081	1.00	127.28	O
ATOM	1871	CB	ASP	A	242	16.509	-16.230	14.128	1.00	134.37	C
ATOM	1872	CG	ASP	A	242	15.076	-15.931	13.693	1.00	137.89	C
ATOM	1873	OD1	ASP	A	242	14.695	-16.306	12.560	1.00	139.91	O
ATOM	1874	OD2	ASP	A	242	14.335	-15.302	14.484	1.00	138.48	O
ATOM	1875	N	GLU	A	243	17.053	-19.614	14.237	1.00	115.47	N
ATOM	1876	CA	GLU	A	243	16.401	-20.892	14.492	1.00	108.81	C
ATOM	1877	C	GLU	A	243	16.219	-21.065	15.984	1.00	101.77	C
ATOM	1878	O	GLU	A	243	15.232	-21.637	16.453	1.00	97.50	O
ATOM	1879	CB	GLU	A	243	17.243	-22.056	13.957	1.00	113.03	C
ATOM	1880	CG	GLU	A	243	18.587	-22.269	14.665	1.00	119.77	C
ATOM	1881	CD	GLU	A	243	19.736	-21.500	14.022	1.00	123.96	C
ATOM	1882	OE1	GLU	A	243	20.004	-21.723	12.821	1.00	128.49	O
ATOM	1883	OE2	GLU	A	243	20.380	-20.682	14.716	1.00	125.21	O
ATOM	1884	N	LYS	A	244	17.193	-20.552	16.719	1.00	90.55	N
ATOM	1885	CA	LYS	A	244	17.196	-20.652	18.159	1.00	87.36	C
ATOM	1886	C	LYS	A	244	16.847	-19.342	18.851	1.00	78.94	C
ATOM	1887	O	LYS	A	244	15.944	-19.299	19.681	1.00	79.48	O
ATOM	1888	CB	LYS	A	244	18.567	-21.157	18.623	1.00	85.94	C
ATOM	1889	CG	LYS	A	244	18.973	-20.687	20.009	1.00	90.77	C
ATOM	1890	CD	LYS	A	244	20.222	-21.392	20.527	1.00	85.35	C
ATOM	1891	CE	LYS	A	244	19.960	-22.872	20.764	1.00	85.15	C
ATOM	1892	NZ	LYS	A	244	18.698	-23.096	21.533	1.00	79.01	N
ATOM	1893	N	HIS	A	245	17.566	-18.279	18.510	1.00	72.67	N
ATOM	1894	CA	HIS	A	245	17.332	-16.978	19.121	1.00	73.65	C
ATOM	1895	C	HIS	A	245	16.275	-16.150	18.398	1.00	71.43	C
ATOM	1896	O	HIS	A	245	16.483	-15.726	17.264	1.00	73.85	O
ATOM	1897	CB	HIS	A	245	18.636	-16.191	19.174	1.00	62.45	C
ATOM	1898	CG	HIS	A	245	19.712	-16.860	19.968	1.00	73.56	C
ATOM	1899	ND1	HIS	A	245	19.566	-17.183	21.301	1.00	75.57	N
ATOM	1900	CD2	HIS	A	245	20.963	-17.251	19.624	1.00	74.25	C
ATOM	1901	CE1	HIS	A	245	20.680	-17.740	21.742	1.00	69.91	C
ATOM	1902	NE2	HIS	A	245	21.542	-17.792	20.747	1.00	78.21	N
ATOM	1903	N	ILE	A	246	15.151	-15.907	19.066	1.00	71.28	N
ATOM	1904	CA	ILE	A	246	14.061	-15.117	18.492	1.00	67.47	C
ATOM	1905	C	ILE	A	246	13.820	-13.823	19.279	1.00	68.54	C
ATOM	1906	O	ILE	A	246	13.465	-13.871	20.459	1.00	56.11	O
ATOM	1907	CB	ILE	A	246	12.746	-15.912	18.494	1.00	71.39	C
ATOM	1908	CG1	ILE	A	246	12.953	-17.270	17.829	1.00	73.66	C
ATOM	1909	CG2	ILE	A	246	11.656	-15.114	17.803	1.00	69.42	C
ATOM	1910	CD1	ILE	A	246	13.544	-17.182	16.451	1.00	82.71	C
ATOM	1911	N	PHE	A	247	13.991	-12.675	18.625	1.00	57.64	N
ATOM	1912	CA	PHE	A	247	13.783	-11.395	19.286	1.00	57.66	C
ATOM	1913	C	PHE	A	247	12.444	-10.766	19.000	1.00	59.75	C

Figure 2 (Table 2 (page 42))

```
ATOM   1914  O    PHE A 247    11.842 -11.003  17.955  1.00 71.91 O
ATOM   1915  CB   PHE A 247    14.831 -10.386  18.866  1.00 58.61 C
ATOM   1916  CG   PHE A 247    16.205 -10.761  19.252  1.00 55.18 C
ATOM   1917  CD1  PHE A 247    16.931 -11.663  18.486  1.00 63.52 C
ATOM   1918  CD2  PHE A 247    16.791 -10.195  20.375  1.00 64.94 C
ATOM   1919  CE1  PHE A 247    18.233 -11.994  18.836  1.00 56.98 C
ATOM   1920  CE2  PHE A 247    18.084 -10.515  20.735  1.00 62.89 C
ATOM   1921  CZ   PHE A 247    18.813 -11.416  19.963  1.00 69.14 C
ATOM   1922  N    SER A 248    11.984  -9.948  19.939  1.00 60.62 N
ATOM   1923  CA   SER A 248    10.741  -9.211  19.761  1.00 59.42 C
ATOM   1924  C    SER A 248    11.135  -8.035  18.848  1.00 58.07 C
ATOM   1925  O    SER A 248    12.324  -7.793  18.605  1.00 50.63 O
ATOM   1926  CB   SER A 248    10.238  -8.684  21.107  1.00 51.67 C
ATOM   1927  OG   SER A 248    11.212  -7.849  21.713  1.00 56.47 O
ATOM   1928  N    ASP A 249    10.156  -7.286  18.364  1.00 62.87 N
ATOM   1929  CA   ASP A 249    10.433  -6.168  17.461  1.00 68.58 C
ATOM   1930  C    ASP A 249    11.414  -5.157  18.016  1.00 71.42 C
ATOM   1931  O    ASP A 249    12.289  -4.649  17.304  1.00 70.32 O
ATOM   1932  CB   ASP A 249     9.113  -5.519  17.102  1.00 78.97 C
ATOM   1933  CG   ASP A 249     8.122  -6.538  16.598  1.00 85.41 C
ATOM   1934  OD1  ASP A 249     8.266  -6.986  15.438  1.00 90.50 O
ATOM   1935  OD2  ASP A 249     7.218  -6.926  17.370  1.00 85.77 O
ATOM   1936  N    ASP A 250    11.274  -4.875  19.297  1.00 71.27 N
ATOM   1937  CA   ASP A 250    12.159  -3.942  19.964  1.00 74.17 C
ATOM   1938  C    ASP A 250    13.358  -4.713  20.521  1.00 70.10 C
ATOM   1939  O    ASP A 250    14.337  -4.113  20.971  1.00 70.84 O
ATOM   1940  CB   ASP A 250    11.390  -3.284  21.100  1.00 82.42 C
ATOM   1941  CG   ASP A 250    10.583  -4.296  21.895  1.00 86.25 C
ATOM   1942  OD1  ASP A 250    10.204  -5.350  21.328  1.00 87.71 O
ATOM   1943  OD2  ASP A 250    10.316  -4.044  23.082  1.00 99.42 O
ATOM   1944  N    SER A 251    13.266  -6.044  20.478  1.00 61.34 N
ATOM   1945  CA   SER A 251    14.301  -6.932  21.005  1.00 60.93 C
ATOM   1946  C    SER A 251    14.357  -6.787  22.529  1.00 55.43 C
ATOM   1947  O    SER A 251    15.398  -6.997  23.149  1.00 54.55 O
ATOM   1948  CB   SER A 251    15.667  -6.615  20.386  1.00 56.47 C
ATOM   1949  OG   SER A 251    15.608  -6.719  18.971  1.00 68.26 O
ATOM   1950  N    SER A 252    13.222  -6.419  23.120  1.00 44.12 N
ATOM   1951  CA   SER A 252    13.132  -6.262  24.565  1.00 54.67 C
ATOM   1952  C    SER A 252    12.961  -7.666  25.142  1.00 45.19 C
ATOM   1953  O    SER A 252    13.231  -7.900  26.321  1.00 45.23 O
ATOM   1954  CB   SER A 252    11.948  -5.359  24.957  1.00 50.26 C
ATOM   1955  OG   SER A 252    10.705  -6.019  24.785  1.00 68.26 O
ATOM   1956  N    GLU A 253    12.511  -8.586  24.288  1.00 39.14 N
ATOM   1957  CA   GLU A 253    12.351  -9.984  24.655  1.00 42.86 C
ATOM   1958  C    GLU A 253    13.245 -10.847  23.787  1.00 55.42 C
ATOM   1959  O    GLU A 253    13.322 -10.649  22.573  1.00 55.46 O
ATOM   1960  CB   GLU A 253    10.924 -10.475  24.459  1.00 46.35 C
ATOM   1961  CG   GLU A 253     9.898  -9.823  25.335  1.00 52.21 C
ATOM   1962  CD   GLU A 253     8.629 -10.640  25.406  1.00 55.68 C
ATOM   1963  OE1  GLU A 253     8.464 -11.550  24.569  1.00 60.84 O
ATOM   1964  OE2  GLU A 253     7.792 -10.370  26.296  1.00 63.61 O
ATOM   1965  N    LEU A 254    13.925 -11.798  24.423  1.00 49.11 N
ATOM   1966  CA   LEU A 254    14.793 -12.741  23.730  1.00 43.78 C
ATOM   1967  C    LEU A 254    14.260 -14.129  24.052  1.00 54.16 C
ATOM   1968  O    LEU A 254    14.179 -14.516  25.221  1.00 49.96 O
ATOM   1969  CB   LEU A 254    16.240 -12.617  24.212  1.00 48.13 C
```

Figure 2 (Table 2 (page 43))

ATOM	1970	CG	LEU	A	254	17.132	-13.793	23.786	1.00	61.15	C
ATOM	1971	CD1	LEU	A	254	17.129	-13.902	22.264	1.00	56.30	C
ATOM	1972	CD2	LEU	A	254	18.561	-13.622	24.314	1.00	45.18	C
ATOM	1973	N	THR	A	255	13.874	-14.873	23.024	1.00	52.09	N
ATOM	1974	CA	THR	A	255	13.343	-16.214	23.233	1.00	55.30	C
ATOM	1975	C	THR	A	255	14.371	-17.254	22.822	1.00	57.05	C
ATOM	1976	O	THR	A	255	14.809	-17.279	21.677	1.00	56.25	O
ATOM	1977	CB	THR	A	255	12.050	-16.444	22.419	1.00	62.05	C
ATOM	1978	OG1	THR	A	255	10.999	-15.630	22.951	1.00	66.84	O
ATOM	1979	CG2	THR	A	255	11.625	-17.908	22.491	1.00	69.28	C
ATOM	1980	N	ILE	A	256	14.784	-18.085	23.774	1.00	57.59	N
ATOM	1981	CA	ILE	A	256	15.740	-19.140	23.482	1.00	53.88	C
ATOM	1982	C	ILE	A	256	14.863	-20.362	23.227	1.00	55.73	C
ATOM	1983	O	ILE	A	256	14.031	-20.740	24.050	1.00	53.74	O
ATOM	1984	CB	ILE	A	256	16.721	-19.325	24.635	1.00	60.39	C
ATOM	1985	CG1	ILE	A	256	17.478	-18.003	24.865	1.00	49.75	C
ATOM	1986	CG2	ILE	A	256	17.729	-20.408	24.263	1.00	67.76	C
ATOM	1987	CD1	ILE	A	256	18.337	-17.959	26.113	1.00	52.15	C
ATOM	1988	N	ARG	A	257	15.049	-20.980	22.070	1.00	60.13	N
ATOM	1989	CA	ARG	A	257	14.153	-22.051	21.657	1.00	71.50	C
ATOM	1990	C	ARG	A	257	14.176	-23.516	22.065	1.00	69.32	C
ATOM	1991	O	ARG	A	257	13.160	-24.049	22.523	1.00	80.18	O
ATOM	1992	CB	ARG	A	257	14.007	-21.955	20.148	1.00	74.93	C
ATOM	1993	CG	ARG	A	257	13.281	-20.678	19.720	1.00	86.48	C
ATOM	1994	CD	ARG	A	257	11.972	-21.046	19.067	1.00	94.98	C
ATOM	1995	NE	ARG	A	257	12.243	-22.177	18.190	1.00	102.55	N
ATOM	1996	CZ	ARG	A	257	11.403	-23.175	17.936	1.00	101.10	C
ATOM	1997	NH1	ARG	A	257	10.194	-23.198	18.481	1.00	98.39	N
ATOM	1998	NH2	ARG	A	257	11.805	-24.190	17.182	1.00	99.09	N
ATOM	1999	N	ASN	A	258	15.287	-24.195	21.864	1.00	61.69	N
ATOM	2000	CA	ASN	A	258	15.340	-25.602	22.253	1.00	64.49	C
ATOM	2001	C	ASN	A	258	16.465	-25.618	23.247	1.00	62.07	C
ATOM	2002	O	ASN	A	258	17.624	-25.892	22.925	1.00	55.85	O
ATOM	2003	CB	ASN	A	258	15.636	-26.481	21.041	1.00	66.15	C
ATOM	2004	CG	ASN	A	258	14.404	-26.716	20.191	1.00	68.75	C
ATOM	2005	OD1	ASN	A	258	13.379	-27.234	20.673	1.00	64.25	O
ATOM	2006	ND2	ASN	A	258	14.484	-26.329	18.926	1.00	70.00	N
ATOM	2007	N	VAL	A	259	16.094	-25.272	24.468	1.00	62.90	N
ATOM	2008	CA	VAL	A	259	17.049	-25.157	25.545	1.00	65.80	C
ATOM	2009	C	VAL	A	259	17.876	-26.384	25.872	1.00	58.88	C
ATOM	2010	O	VAL	A	259	17.365	-27.483	26.054	1.00	56.71	O
ATOM	2011	CB	VAL	A	259	16.370	-24.703	26.858	1.00	64.49	C
ATOM	2012	CG1	VAL	A	259	17.433	-24.328	27.883	1.00	63.04	C
ATOM	2013	CG2	VAL	A	259	15.437	-23.546	26.599	1.00	62.50	C
ATOM	2014	N	ASP	A	260	19.176	-26.159	25.951	1.00	60.37	N
ATOM	2015	CA	ASP	A	260	20.110	-27.191	26.329	1.00	64.76	C
ATOM	2016	C	ASP	A	260	21.141	-26.491	27.190	1.00	63.70	C
ATOM	2017	O	ASP	A	260	21.185	-25.257	27.253	1.00	55.60	O
ATOM	2018	CB	ASP	A	260	20.785	-27.829	25.120	1.00	61.25	C
ATOM	2019	CG	ASP	A	260	21.602	-26.844	24.322	1.00	68.49	C
ATOM	2020	OD1	ASP	A	260	22.091	-25.847	24.896	1.00	68.44	O
ATOM	2021	OD2	ASP	A	260	21.775	-27.084	23.110	1.00	81.31	O
ATOM	2022	N	LYS	A	261	21.986	-27.277	27.832	1.00	57.12	N
ATOM	2023	CA	LYS	A	261	22.985	-26.711	28.711	1.00	51.64	C
ATOM	2024	C	LYS	A	261	23.832	-25.591	28.141	1.00	46.97	C
ATOM	2025	O	LYS	A	261	24.335	-24.757	28.895	1.00	48.66	O

Figure 2 (Table 2 (page 44))

```
ATOM   2026  CB  LYS A 261     23.874 -27.828  29.258  1.00 52.71  C
ATOM   2027  CG  LYS A 261     23.193 -28.612  30.358  1.00 61.87  C
ATOM   2028  CD  LYS A 261     24.105 -29.669  30.947  1.00 73.37  C
ATOM   2029  CE  LYS A 261     23.600 -30.117  32.308  1.00 76.85  C
ATOM   2030  NZ  LYS A 261     23.680 -29.007  33.304  1.00 77.99  N
ATOM   2031  N   ASN A 262     24.004 -25.534  26.827  1.00 51.62  N
ATOM   2032  CA  ASN A 262     24.834 -24.464  26.278  1.00 50.71  C
ATOM   2033  C   ASN A 262     24.189 -23.099  26.414  1.00 49.52  C
ATOM   2034  O   ASN A 262     24.835 -22.073  26.224  1.00 44.29  O
ATOM   2035  CB  ASN A 262     25.160 -24.707  24.815  1.00 63.69  C
ATOM   2036  CG  ASN A 262     26.545 -25.256  24.636  1.00 76.99  C
ATOM   2037  OD1 ASN A 262     27.466 -24.881  25.368  1.00 88.03  O
ATOM   2038  ND2 ASN A 262     26.713 -26.145  23.664  1.00 83.71  N
ATOM   2039  N   ASP A 263     22.911 -23.100  26.755  1.00 43.87  N
ATOM   2040  CA  ASP A 263     22.173 -21.864  26.915  1.00 49.29  C
ATOM   2041  C   ASP A 263     22.341 -21.257  28.307  1.00 56.55  C
ATOM   2042  O   ASP A 263     21.984 -20.103  28.532  1.00 45.77  O
ATOM   2043  CB  ASP A 263     20.705 -22.115  26.593  1.00 46.15  C
ATOM   2044  CG  ASP A 263     20.502 -22.558  25.148  1.00 47.16  C
ATOM   2045  OD1 ASP A 263     21.208 -22.006  24.272  1.00 50.06  O
ATOM   2046  OD2 ASP A 263     19.642 -23.440  24.894  1.00 53.96  O
ATOM   2047  N   GLU A 264     22.886 -22.033  29.241  1.00 52.20  N
ATOM   2048  CA  GLU A 264     23.126 -21.517  30.580  1.00 50.47  C
ATOM   2049  C   GLU A 264     24.217 -20.455  30.464  1.00 55.25  C
ATOM   2050  O   GLU A 264     25.286 -20.722  29.917  1.00 51.52  O
ATOM   2051  CB  GLU A 264     23.575 -22.644  31.526  1.00 49.18  C
ATOM   2052  CG  GLU A 264     23.865 -22.150  32.948  1.00 56.13  C
ATOM   2053  CD  GLU A 264     24.070 -23.270  33.968  1.00 59.96  C
ATOM   2054  OE1 GLU A 264     23.144 -24.088  34.166  1.00 52.27  O
ATOM   2055  OE2 GLU A 264     25.161 -23.319  34.575  1.00 63.96  O
ATOM   2056  N   ALA A 265     23.936 -19.254  30.971  1.00 50.58  N
ATOM   2057  CA  ALA A 265     24.882 -18.143  30.932  1.00 49.56  C
ATOM   2058  C   ALA A 265     24.285 -16.892  31.553  1.00 44.28  C
ATOM   2059  O   ALA A 265     23.138 -16.876  32.020  1.00 44.60  O
ATOM   2060  CB  ALA A 265     25.275 -17.839  29.485  1.00 55.17  C
ATOM   2061  N   GLU A 266     25.084 -15.837  31.565  1.00 46.95  N
ATOM   2062  CA  GLU A 266     24.597 -14.566  32.052  1.00 58.95  C
ATOM   2063  C   GLU A 266     24.233 -13.782  30.796  1.00 54.06  C
ATOM   2064  O   GLU A 266     25.077 -13.547  29.937  1.00 49.16  O
ATOM   2065  CB  GLU A 266     25.662 -13.784  32.824  1.00 49.59  C
ATOM   2066  CG  GLU A 266     25.188 -12.371  33.185  1.00 68.76  C
ATOM   2067  CD  GLU A 266     26.312 -11.461  33.655  1.00 79.04  C
ATOM   2068  OE1 GLU A 266     27.442 -11.585  33.135  1.00 92.30  O
ATOM   2069  OE2 GLU A 266     26.071 -10.604  34.534  1.00 84.00  O
ATOM   2070  N   TYR A 267     22.969 -13.405  30.682  1.00 56.50  N
ATOM   2071  CA  TYR A 267     22.539 -12.620  29.539  1.00 53.55  C
ATOM   2072  C   TYR A 267     22.379 -11.175  29.973  1.00 53.33  C
ATOM   2073  O   TYR A 267     21.857 -10.899  31.051  1.00 56.26  O
ATOM   2074  CB  TYR A 267     21.216 -13.131  29.000  1.00 41.05  C
ATOM   2075  CG  TYR A 267     21.302 -14.503  28.392  1.00 52.19  C
ATOM   2076  CD1 TYR A 267     21.310 -15.645  29.200  1.00 46.18  C
ATOM   2077  CD2 TYR A 267     21.374 -14.669  27.010  1.00 42.85  C
ATOM   2078  CE1 TYR A 267     21.385 -16.907  28.649  1.00 36.41  C
ATOM   2079  CE2 TYR A 267     21.447 -15.926  26.447  1.00 47.87  C
ATOM   2080  CZ  TYR A 267     21.454 -17.043  27.269  1.00 46.20  C
ATOM   2081  OH  TYR A 267     21.534 -18.289  26.709  1.00 46.42  O
```

Figure 2 (Table 2 (page 45))

ATOM	2082	N	VAL	A	268	22.849	-10.259	29.134	1.00 54.55	N
ATOM	2083	CA	VAL	A	268	22.744	-8.833	29.420	1.00 51.27	C
ATOM	2084	C	VAL	A	268	21.939	-8.121	28.325	1.00 53.04	C
ATOM	2085	O	VAL	A	268	22.238	-8.268	27.140	1.00 49.32	O
ATOM	2086	CB	VAL	A	268	24.149	-8.164	29.507	1.00 51.72	C
ATOM	2087	CG1	VAL	A	268	24.008	-6.653	29.697	1.00 53.25	C
ATOM	2088	CG2	VAL	A	268	24.954	-8.757	30.667	1.00 53.72	C
ATOM	2089	N	CYS	A	269	20.909	-7.372	28.708	1.00 47.02	N
ATOM	2090	CA	CYS	A	269	20.130	-6.631	27.712	1.00 46.07	C
ATOM	2091	C	CYS	A	269	20.572	-5.192	27.825	1.00 48.28	C
ATOM	2092	O	CYS	A	269	20.513	-4.568	28.893	1.00 54.75	O
ATOM	2093	CB	CYS	A	269	18.645	-6.725	27.972	1.00 47.89	C
ATOM	2094	SG	CYS	A	269	18.154	-6.060	29.588	1.00 57.20	S
ATOM	2095	N	ILE	A	270	21.040	-4.684	26.705	1.00 44.49	N
ATOM	2096	CA	ILE	A	270	21.542	-3.334	26.618	1.00 54.21	C
ATOM	2097	C	ILE	A	270	20.492	-2.429	25.984	1.00 51.98	C
ATOM	2098	O	ILE	A	270	20.057	-2.665	24.858	1.00 52.39	O
ATOM	2099	CB	ILE	A	270	22.804	-3.333	25.757	1.00 58.16	C
ATOM	2100	CG1	ILE	A	270	23.777	-4.385	26.287	1.00 59.14	C
ATOM	2101	CG2	ILE	A	270	23.451	-1.964	25.768	1.00 58.07	C
ATOM	2102	CD1	ILE	A	270	24.907	-4.698	25.332	1.00 62.65	C
ATOM	2103	N	ALA	A	271	20.068	-1.413	26.725	1.00 46.08	N
ATOM	2104	CA	ALA	A	271	19.081	-0.463	26.220	1.00 43.82	C
ATOM	2105	C	ALA	A	271	19.811	0.838	25.863	1.00 41.91	C
ATOM	2106	O	ALA	A	271	20.461	1.454	26.713	1.00 41.51	O
ATOM	2107	CB	ALA	A	271	18.010	-0.212	27.272	1.00 40.50	C
ATOM	2108	N	GLU	A	272	19.709	1.242	24.601	1.00 43.98	N
ATOM	2109	CA	GLU	A	272	20.375	2.453	24.128	1.00 50.40	C
ATOM	2110	C	GLU	A	272	19.526	3.346	23.255	1.00 40.39	C
ATOM	2111	O	GLU	A	272	18.635	2.880	22.548	1.00 43.66	O
ATOM	2112	CB	GLU	A	272	21.589	2.115	23.251	1.00 46.89	C
ATOM	2113	CG	GLU	A	272	22.738	1.366	23.863	1.00 76.32	C
ATOM	2114	CD	GLU	A	272	23.835	1.101	22.832	1.00 88.35	C
ATOM	2115	OE1	GLU	A	272	23.496	0.886	21.643	1.00 95.66	O
ATOM	2116	OE2	GLU	A	272	25.031	1.096	23.206	1.00 91.47	O
ATOM	2117	N	ASN	A	273	19.843	4.635	23.316	1.00 46.76	N
ATOM	2118	CA	ASN	A	273	19.260	5.648	22.438	1.00 47.59	C
ATOM	2119	C	ASN	A	273	20.335	6.718	22.340	1.00 52.11	C
ATOM	2120	O	ASN	A	273	21.366	6.622	23.008	1.00 44.76	O
ATOM	2121	CB	ASN	A	273	17.897	6.201	22.916	1.00 46.27	C
ATOM	2122	CG	ASN	A	273	17.964	6.980	24.211	1.00 44.51	C
ATOM	2123	OD1	ASN	A	273	19.012	7.471	24.611	1.00 44.37	O
ATOM	2124	ND2	ASN	A	273	16.808	7.126	24.866	1.00 38.00	N
ATOM	2125	N	LYS	A	274	20.128	7.723	21.504	1.00 56.80	N
ATOM	2126	CA	LYS	A	274	21.154	8.740	21.317	1.00 51.83	C
ATOM	2127	C	LYS	A	274	21.618	9.485	22.567	1.00 54.11	C
ATOM	2128	O	LYS	A	274	22.667	10.123	22.545	1.00 58.51	O
ATOM	2129	CB	LYS	A	274	20.718	9.742	20.238	1.00 55.02	C
ATOM	2130	CG	LYS	A	274	19.590	10.658	20.644	1.00 47.96	C
ATOM	2131	CD	LYS	A	274	18.892	11.218	19.403	1.00 52.54	C
ATOM	2132	CE	LYS	A	274	19.784	12.175	18.622	1.00 65.50	C
ATOM	2133	NZ	LYS	A	274	19.120	12.652	17.364	1.00 68.41	N
ATOM	2134	N	ALA	A	275	20.869	9.403	23.659	1.00 47.65	N
ATOM	2135	CA	ALA	A	275	21.275	10.100	24.868	1.00 48.41	C
ATOM	2136	C	ALA	A	275	21.944	9.233	25.930	1.00 49.48	C
ATOM	2137	O	ALA	A	275	22.294	9.735	26.988	1.00 50.34	O

Figure 2 (Table 2 (page 46))

ATOM	2138	CB	ALA	A	275	20.084	10.814	25.487	1.00 44.55	C
ATOM	2139	N	GLY	A	276	22.122	7.942	25.691	1.00 49.34	N
ATOM	2140	CA	GLY	A	276	22.755	7.177	26.746	1.00 51.88	C
ATOM	2141	C	GLY	A	276	22.482	5.694	26.738	1.00 50.21	C
ATOM	2142	O	GLY	A	276	21.907	5.164	25.779	1.00 51.48	O
ATOM	2143	N	GLU	A	277	22.868	5.026	27.824	1.00 50.99	N
ATOM	2144	CA	GLU	A	277	22.696	3.586	27.906	1.00 53.05	C
ATOM	2145	C	GLU	A	277	22.598	3.056	29.316	1.00 51.11	C
ATOM	2146	O	GLU	A	277	23.116	3.655	30.249	1.00 52.32	O
ATOM	2147	CB	GLU	A	277	23.873	2.915	27.194	1.00 58.98	C
ATOM	2148	CG	GLU	A	277	23.900	1.389	27.218	1.00 74.31	C
ATOM	2149	CD	GLU	A	277	24.570	0.797	28.462	1.00 89.46	C
ATOM	2150	OE1	GLU	A	277	25.277	1.537	29.183	1.00 96.28	O
ATOM	2151	OE2	GLU	A	277	24.398	-0.420	28.705	1.00 89.19	O
ATOM	2152	N	GLN	A	278	21.907	1.927	29.453	1.00 49.66	N
ATOM	2153	CA	GLN	A	278	21.783	1.228	30.724	1.00 45.13	C
ATOM	2154	C	GLN	A	278	21.513	-0.239	30.415	1.00 50.42	C
ATOM	2155	O	GLN	A	278	20.877	-0.568	29.417	1.00 46.75	O
ATOM	2156	CB	GLN	A	278	20.662	1.789	31.607	1.00 48.09	C
ATOM	2157	CG	GLN	A	278	20.812	1.327	33.064	1.00 46.69	C
ATOM	2158	CD	GLN	A	278	19.700	1.822	33.976	1.00 57.97	C
ATOM	2159	OE1	GLN	A	278	18.572	1.330	33.917	1.00 44.46	O
ATOM	2160	NE2	GLN	A	278	20.012	2.800	34.826	1.00 53.33	N
ATOM	2161	N	ASP	A	279	22.013	-1.132	31.257	1.00 45.92	N
ATOM	2162	CA	ASP	A	279	21.795	-2.541	31.014	1.00 47.69	C
ATOM	2163	C	ASP	A	279	21.345	-3.251	32.270	1.00 47.71	C
ATOM	2164	O	ASP	A	279	21.357	-2.687	33.366	1.00 48.35	O
ATOM	2165	CB	ASP	A	279	23.062	-3.186	30.451	1.00 60.02	C
ATOM	2166	CG	ASP	A	279	24.316	-2.707	31.154	1.00 69.17	C
ATOM	2167	OD1	ASP	A	279	24.456	-2.954	32.370	1.00 75.17	O
ATOM	2168	OD2	ASP	A	279	25.157	-2.073	30.490	1.00 75.70	O
ATOM	2169	N	ALA	A	280	20.892	-4.480	32.079	1.00 49.27	N
ATOM	2170	CA	ALA	A	280	20.428	-5.314	33.172	1.00 57.28	C
ATOM	2171	C	ALA	A	280	20.804	-6.748	32.833	1.00 54.10	C
ATOM	2172	O	ALA	A	280	20.868	-7.126	31.659	1.00 47.63	O
ATOM	2173	CB	ALA	A	280	18.909	-5.184	33.341	1.00 47.77	C
ATOM	2174	N	SER	A	281	21.043	-7.560	33.854	1.00 53.68	N
ATOM	2175	CA	SER	A	281	21.429	-8.931	33.599	1.00 48.69	C
ATOM	2176	C	SER	A	281	20.402	-9.952	34.031	1.00 45.20	C
ATOM	2177	O	SER	A	281	19.595	-9.718	34.934	1.00 45.89	O
ATOM	2178	CB	SER	A	281	22.768	-9.219	34.279	1.00 61.38	C
ATOM	2179	OG	SER	A	281	22.718	-8.863	35.646	1.00 57.59	O
ATOM	2180	N	ILE	A	282	20.427	-11.086	33.349	1.00 43.38	N
ATOM	2181	CA	ILE	A	282	19.524	-12.185	33.637	1.00 41.38	C
ATOM	2182	C	ILE	A	282	20.392	-13.429	·33.671	1.00 47.86	C
ATOM	2183	O	ILE	A	282	21.235	-13.631	32.799	1.00 51.03	O
ATOM	2184	CB	ILE	A	282	18.436	-12.316	32.548	1.00 40.14	C
ATOM	2185	CG1	ILE	A	282	17.557	-11.056	32.557	1.00 46.94	C
ATOM	2186	CG2	ILE	A	282	17.576	-13.549	32.807	1.00 42.53	C
ATOM	2187	CD1	ILE	A	282	16.484	-10.998	31.476	1.00 45.40	C
ATOM	2188	N	HIS	A	283	20.204	-14.248	34.695	1.00 45.39	N
ATOM	2189	CA	HIS	A	283	20.998	-15.458	34.816	1.00 46.01	C
ATOM	2190	C	HIS	A	283	20.145	-16.651	34.501	1.00 41.84	C
ATOM	2191	O	HIS	A	283	19.164	-16.923	35.197	1.00 51.27	O
ATOM	2192	CB	HIS	A	283	21.570	-15.575	36.230	1.00 53.96	C
ATOM	2193	CG	HIS	A	283	22.617	-14.551	36.543	1.00 60.28	C

Figure 2 (Table 2 (page 47))

```
ATOM    2194  ND1 HIS A 283    23.908 -14.633  36.065  1.00 69.25  N
ATOM    2195  CD2 HIS A 283    22.554 -13.401  37.260  1.00 68.71  C
ATOM    2196  CE1 HIS A 283    24.593 -13.578  36.473  1.00 75.43  C
ATOM    2197  NE2 HIS A 283    23.796 -12.816  37.199  1.00 66.88  N
ATOM    2198  N   LEU A 284    20.499 -17.349  33.427  1.00 41.70  N
ATOM    2199  CA  LEU A 284    19.752 -18.534  33.050  1.00 45.86  C
ATOM    2200  C   LEU A 284    20.533 -19.778  33.469  1.00 49.53  C
ATOM    2201  O   LEU A 284    21.683 -19.963  33.058  1.00 45.44  O
ATOM    2202  CB  LEU A 284    19.515 -18.576  31.532  1.00 41.74  C
ATOM    2203  CG  LEU A 284    18.782 -19.827  31.028  1.00 47.91  C
ATOM    2204  CD1 LEU A 284    17.407 -19.888  31.680  1.00 45.59  C
ATOM    2205  CD2 LEU A 284    18.648 -19.810  29.500  1.00 48.70  C
ATOM    2206  N   LYS A 285    19.913 -20.625  34.285  1.00 48.59  N
ATOM    2207  CA  LYS A 285    20.557 -21.863  34.711  1.00 53.60  C
ATOM    2208  C   LYS A 285    19.797 -23.008  34.061  1.00 46.75  C
ATOM    2209  O   LYS A 285    18.570 -23.061  34.109  1.00 49.33  O
ATOM    2210  CB  LYS A 285    20.531 -21.991  36.239  1.00 56.58  C
ATOM    2211  CG  LYS A 285    21.302 -20.880  36.942  1.00 63.01  C
ATOM    2212  CD  LYS A 285    21.254 -21.021  38.459  1.00 71.05  C
ATOM    2213  CE  LYS A 285    21.853 -19.795  39.148  1.00 76.77  C
ATOM    2214  NZ  LYS A 285    20.993 -18.583  39.020  1.00 73.22  N
ATOM    2215  N   VAL A 286    20.525 -23.922  33.436  1.00 44.47  N
ATOM    2216  CA  VAL A 286    19.888 -25.047  32.759  1.00 53.73  C
ATOM    2217  C   VAL A 286    20.271 -26.367  33.410  1.00 58.55  C
ATOM    2218  O   VAL A 286    21.446 -26.709  33.489  1.00 58.02  O
ATOM    2219  CB  VAL A 286    20.283 -25.078  31.268  1.00 49.11  C
ATOM    2220  CG1 VAL A 286    19.618 -26.248  30.572  1.00 52.83  C
ATOM    2221  CG2 VAL A 286    19.872 -23.760  30.597  1.00 49.45  C
ATOM    2222  N   PHE A 287    19.267 -27.100  33.875  1.00 56.62  N
ATOM    2223  CA  PHE A 287    19.493 -28.379  34.528  1.00 60.81  C
ATOM    2224  C   PHE A 287    19.172 -29.540  33.607  1.00 64.78  C
ATOM    2225  O   PHE A 287    18.208 -29.487  32.846  1.00 64.16  O
ATOM    2226  CB  PHE A 287    18.645 -28.461  35.795  1.00 58.95  C
ATOM    2227  CG  PHE A 287    18.868 -27.314  36.724  1.00 61.24  C
ATOM    2228  CD1 PHE A 287    17.963 -26.259  36.783  1.00 56.19  C
ATOM    2229  CD2 PHE A 287    20.036 -27.237  37.477  1.00 62.69  C
ATOM    2230  CE1 PHE A 287    18.224 -25.139  37.575  1.00 53.03  C
ATOM    2231  CE2 PHE A 287    20.304 -26.124  38.266  1.00 58.31  C
ATOM    2232  CZ  PHE A 287    19.397 -25.073  38.314  1.00 59.07  C
ATOM    2233  N   ALA A 288    19.997 -30.583  33.666  1.00 66.33  N
ATOM    2234  CA  ALA A 288    19.795 -31.766  32.834  1.00 73.18  C
ATOM    2235  C   ALA A 288    18.428 -32.377  33.119  1.00 78.08  C
ATOM    2236  O   ALA A 288    17.960 -32.349  34.259  1.00 78.39  O
ATOM    2237  CB  ALA A 288    20.887 -32.785  33.106  1.00 69.96  C
ATOM    2238  N   LYS A 289    17.794 -32.931  32.087  1.00 80.55  N
ATOM    2239  CA  LYS A 289    16.476 -33.541  32.240  1.00 84.08  C
ATOM    2240  C   LYS A 289    16.535 -34.855  33.016  1.00 88.56  C
ATOM    2241  O   LYS A 289    15.585 -35.127  33.785  1.00 92.60  O
ATOM    2242  CB  LYS A 289    15.830 -33.779  30.872  1.00 82.11  C
ATOM    2243  CG  LYS A 289    16.538 -34.804  30.009  1.00 82.83  C
ATOM    2244  CD  LYS A 289    15.739 -35.066  28.748  1.00 81.13  C
ATOM    2245  CE  LYS A 289    16.362 -36.164  27.910  1.00 87.98  C
ATOM    2246  NZ  LYS A 289    15.562 -36.424  26.677  1.00 90.82  N
ATOM    2247  OXT LYS A 289    17.519 -35.608  32.835  1.00 94.14  O
TER     2248      LYS A 289
HETATM  2249  O   HOH     1    26.862  53.829  -2.499  1.00 53.80  O
```

Figure 2 (Table 2 (page 48))

```
HETATM 2250  O   HOH    2    31.435  56.206   -5.661  1.00  53.53  O
HETATM 2251  O   HOH    4    18.815  60.633  -12.908  1.00  43.98  O
HETATM 2252  O   HOH    5    16.291  34.157    5.585  1.00  64.41  O
HETATM 2253  O   HOH    6    24.283  23.825   11.233  1.00  59.48  O
HETATM 2254  O   HOH    7    21.204  19.365   17.749  1.00  60.83  O
HETATM 2255  O   HOH    8    15.430  12.803   19.226  1.00  45.67  O
HETATM 2256  O   HOH    9    22.245  15.815   31.410  1.00  50.19  O
HETATM 2257  O   HOH   10    25.429  21.325   30.709  1.00  49.37  O
HETATM 2258  O   HOH   11    23.048  36.010   15.248  1.00  51.13  O
HETATM 2259  O   HOH   12    29.692  33.165   19.866  1.00  37.03  O
HETATM 2260  O   HOH   13     9.169  23.139   31.247  1.00  61.40  O
HETATM 2261  O   HOH   14    17.022  56.166    8.038  1.00  75.27  O
HETATM 2262  O   HOH   15     8.769  40.002    7.174  1.00  48.91  O
HETATM 2263  O   HOH   16    10.231  43.238    7.473  1.00  47.42  O
HETATM 2264  O   HOH   17    15.641  26.081    5.720  1.00  78.13  O
HETATM 2265  O   HOH   18    20.551  14.627   22.658  1.00  46.05  O
HETATM 2266  O   HOH   19    11.221  -2.472   26.804  1.00  52.85  O
HETATM 2267  O   HOH   20    13.041  60.224   -4.320  1.00  64.49  O
HETATM 2268  O   HOH   21    14.835  48.897   -2.048  1.00  85.96  O
HETATM 2269  O   HOH   22    29.546  51.498  -21.147  1.00  47.61  O
HETATM 2270  O   HOH   23    24.511  42.141  -28.698  1.00  76.55  O
HETATM 2271  O   HOH   25    21.636  45.365  -18.499  1.00  37.40  O
HETATM 2272  O   HOH   26    15.790  47.805  -19.728  1.00  64.11  O
HETATM 2273  O   HOH   27    20.999  58.533   -6.980  1.00  47.49  O
HETATM 2274  O   HOH   28    14.534  40.436    5.659  1.00  59.32  O
HETATM 2275  O   HOH   29    18.746  16.322   14.473  1.00  79.28  O
HETATM 2276  O   HOH   30    25.965  40.212    9.533  1.00  52.16  O
HETATM 2277  O   HOH   31    16.482  55.396   13.144  1.00  59.76  O
HETATM 2278  O   HOH   32     9.922  15.732   20.883  1.00  48.37  O
HETATM 2279  O   HOH   33    11.915  -0.137   41.445  1.00  73.91  O
HETATM 2280  O   HOH   34    11.044   7.531   19.815  1.00  49.89  O
HETATM 2281  O   HOH   35     6.902   3.742   25.922  1.00  63.36  O
HETATM 2282  O   HOH   37    21.399  -1.338   20.994  1.00  76.17  O
HETATM 2283  O   HOH   38    18.329  53.773   -1.977  1.00  62.61  O
HETATM 2284  O   HOH   39    18.014  43.718   -2.937  1.00  49.73  O
HETATM 2285  O   HOH   40    32.281  40.568  -12.177  1.00  66.60  O
HETATM 2286  O   HOH   41    19.381  44.469  -19.805  1.00  64.16  O
HETATM 2287  O   HOH   42    25.046  41.566  -20.577  1.00  61.50  O
HETATM 2288  O   HOH   46     7.104   2.690   28.661  1.00  90.82  O
HETATM 2289  O   HOH   48    29.774 -14.171   32.170  1.00  72.60  O
HETATM 2290  O   HOH   49    36.677  48.530  -18.261  1.00  57.32  O
HETATM 2291  O   HOH   50    33.317  46.204  -17.946  1.00  47.09  O
HETATM 2292  O   HOH   52    22.357  37.802   16.682  1.00  62.95  O
HETATM 2293  O   HOH   54    11.598   9.583   18.307  1.00  51.71  O
HETATM 2294  O   HOH   55    22.448  12.959   33.086  1.00  71.24  O
HETATM 2295  O   HOH   56    12.323 -25.457   30.778  1.00  69.54  O
HETATM 2296  O   HOH   57    22.080  16.779   21.536  1.00  49.07  O
HETATM 2297  O   HOH   58    17.068   4.212   19.556  1.00  71.54  O
HETATM 2298  O   HOH   59    21.824  23.695   19.290  1.00  44.38  O
HETATM 2299  O   HOH   60    17.965   7.263   19.831  1.00  45.41  O
HETATM 2300  O   HOH   61    19.593  -1.710   35.113  1.00  49.69  O
HETATM 2301  O   HOH   62    18.642  -7.793   36.955  1.00  68.54  O
HETATM 2302  O   HOH   63    23.848  -0.227   33.498  1.00  54.90  O
HETATM 2303  O   HOH   64    31.052 -17.541   34.986  1.00  68.80  O
HETATM 2304  O   HOH   65     5.551  -4.238    9.968  1.00  64.86  O
HETATM 2305  O   HOH   66    10.472  -3.423    9.588  1.00  81.77  O
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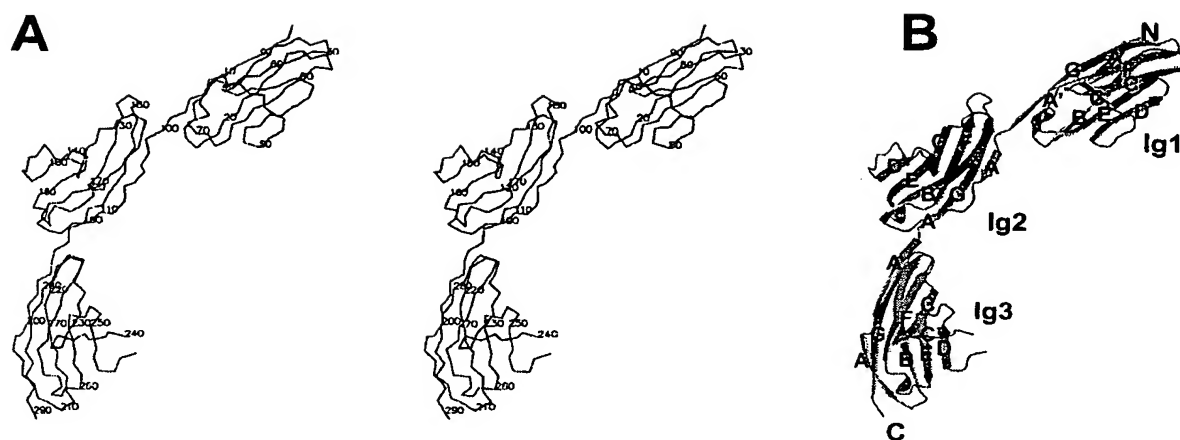
Figure 2 (Table 2 (page 49))

HETATM	2306	O	HOH	67	6.705	-3.198	12.269	1.00 59.36	O
HETATM	2307	O	HOH	68	18.934	8.523	16.255	1.00 70.67	O
HETATM	2308	O	HOH	69	26.373	-11.223	28.910	1.00 53.04	O
HETATM	2309	O	HOH	70	26.631	6.184	27.729	1.00 74.30	O
HETATM	2310	O	HOH	71	26.466	-20.918	34.876	1.00 70.68	O
HETATM	2311	O	HOH	72	8.293	12.647	18.395	1.00 56.61	O
HETATM	2312	O	HOH	74	17.106	-5.693	36.496	1.00 48.96	O
HETATM	2313	O	HOH	75	1.311	-8.583	8.383	1.00 70.05	O
HETATM	2314	O	HOH	76	26.233	40.015	4.081	1.00 64.69	O
HETATM	2315	O	HOH	77	21.018	39.423	0.780	1.00 63.73	O
HETATM	2316	O	HOH	78	30.385	47.077	-9.984	1.00 47.01	O
HETATM	2317	O	HOH	80	17.757	22.465	9.580	1.00 54.37	O
HETATM	2318	O	HOH	81	25.847	39.446	18.635	1.00 61.83	O
HETATM	2319	O	HOH	82	23.903	-18.248	35.163	1.00 66.46	O
HETATM	2320	O	HOH	83	17.550	29.059	7.625	1.00 69.50	O
HETATM	2321	O	HOH	84	22.192	30.581	38.779	1.00 45.18	O
HETATM	2322	O	HOH	85	19.724	26.758	8.865	1.00 62.11	O
HETATM	2323	O	HOH	87	29.601	58.691	-24.045	1.00 49.94	O
HETATM	2324	O	HOH	88	22.701	60.581	-7.832	1.00 65.08	O
HETATM	2325	O	HOH	89	21.940	62.739	-12.104	1.00 60.23	O
HETATM	2326	O	HOH	90	28.142	44.638	-19.542	1.00 52.86	O
HETATM	2327	O	HOH	91	19.926	59.567	-10.713	1.00 54.05	O
HETATM	2328	O	HOH	92	23.841	23.097	24.364	1.00 55.20	O
HETATM	2329	O	HOH	93	14.026	37.104	24.024	1.00 50.35	O
HETATM	2330	O	HOH	94	28.637	30.316	16.747	1.00 47.63	O
HETATM	2331	O	HOH	95	13.597	-12.079	32.292	1.00 47.38	O
HETATM	2332	O	HOH	96	20.525	6.030	31.726	1.00 59.12	O
HETATM	2333	O	HOH	97	12.219	25.294	38.142	1.00 74.46	O
HETATM	2334	O	HOH	98	17.582	46.166	-21.327	1.00 58.26	O
HETATM	2335	O	HOH	99	18.462	3.098	17.614	1.00 74.29	O
HETATM	2336	O	HOH	100	7.657	-6.217	21.068	1.00 54.31	O
HETATM	2337	O	HOH	101	31.973	58.468	-22.566	1.00 51.37	O
HETATM	2338	O	HOH	102	25.581	34.891	15.303	1.00 62.92	O
HETATM	2339	O	HOH	103	9.781	4.793	26.865	1.00 52.97	O
HETATM	2340	O	HOH	104	27.113	28.768	14.346	1.00 46.27	O
HETATM	2341	O	HOH	105	20.934	59.591	-4.081	1.00 63.10	O
HETATM	2342	O	HOH	106	29.101	39.039	-6.576	1.00 50.94	O
HETATM	2343	O	HOH	107	20.829	-6.266	36.888	1.00 67.77	O
HETATM	2344	O	HOH	108	14.801	-6.395	38.213	1.00 57.81	O
HETATM	2345	O	HOH	109	21.412	-19.178	24.173	1.00 57.65	O
HETATM	2346	O	HOH	110	29.742	32.206	15.564	1.00 51.50	O
HETATM	2347	O	HOH	111	27.197	38.482	-3.772	1.00 57.43	O
HETATM	2348	O	HOH	112	23.730	20.567	24.733	1.00 63.78	O
HETATM	2349	O	HOH	113	15.996	50.339	-4.519	1.00 68.59	O
HETATM	2350	O	HOH	114	10.665	-4.867	34.503	1.00 53.34	O
HETATM	2351	O	HOH	115	6.955	17.535	26.540	1.00 72.17	O
HETATM	2352	O	HOH	116	15.712	-29.078	24.014	1.00 65.77	O
HETATM	2353	O	HOH	118	32.255	44.366	-7.537	1.00 62.15	O
HETATM	2354	O	HOH	119	29.827	41.068	-0.664	1.00 57.67	O
HETATM	2355	O	HOH	122	14.630	-27.859	26.706	1.00 65.41	O
HETATM	2356	O	HOH	123	8.521	-18.764	25.803	1.00 74.48	O
HETATM	2357	O	HOH	125	15.199	60.049	-12.759	1.00 63.41	O
HETATM	2358	O	HOH	126	10.378	14.473	18.707	1.00 52.05	O
HETATM	2359	O	HOH	127	28.187	-10.553	30.862	1.00 65.81	O
HETATM	2360	O	HOH	128	7.837	37.705	8.662	1.00 62.54	O
HETATM	2361	O	HOH	130	23.744	37.155	1.565	1.00 65.13	O

Figure 2 (Table 2 (page 50))

```
HETATM 2362  O   HOH   131    13.354  57.052  -9.380  1.00  64.16  O
HETATM 2363  O   HOH   132    31.235  44.417 -16.467  1.00  58.09  O
HETATM 2364  O   HOH   134    18.966  44.757   7.268  1.00  51.54  O
HETATM 2365  O   HOH   135    22.888   3.287  35.759  1.00  66.29  O
HETATM 2366  O   HOH   136    10.345  29.244  10.371  1.00  53.80  O
HETATM 2367  O   HOH   137    21.314  -8.331  20.298  1.00  59.91  O
HETATM 2368  O   HOH   138    38.747  55.169 -17.210  1.00  61.68  O
HETATM 2369  O   HOH   139    14.760  55.271  10.174  1.00  55.52  O
HETATM 2370  O   HOH   140    23.711  55.591   3.512  1.00  78.73  O
HETATM 2371  O   HOH   142     5.285  37.922   7.977  1.00  63.10  O
HETATM 2372  O   HOH   143    24.355  15.578  30.186  1.00  68.63  O
HETATM 2373  O   HOH   144    23.201   9.987  31.463  1.00  64.84  O
HETATM 2374  O   HOH   145    15.111  -8.434  40.304  1.00  70.85  O
HETATM 2375  O   HOH   146    34.105  49.705  -9.362  1.00  66.43  O
HETATM 2376  O   HOH   147    22.545  50.730   2.853  1.00  70.28  O
HETATM 2377  O   HOH   149    23.888  38.804 -17.868  1.00  69.84  O
HETATM 2378  O   HOH   150    26.301  66.907 -32.270  1.00  69.82  O
HETATM 2379  O   HOH   151    29.578  51.924 -24.078  1.00  67.26  O
HETATM 2380  O   HOH   152    31.935  49.759  -6.982  1.00  72.11  O
HETATM 2381  O   HOH   153    11.771  12.964  31.927  1.00  70.57  O
HETATM 2382  O   HOH   154    14.696   6.619  31.148  1.00  64.86  O
HETATM 2383  O   HOH   155    33.398  69.714 -31.980  1.00  74.81  O
HETATM 2384  O   HOH   156    26.480  50.982   0.230  1.00  59.10  O
HETATM 2385  O   HOH   157    22.798   7.195  30.848  1.00  68.26  O
HETATM 2386  O   HOH   158    19.477  -6.906  18.703  1.00  72.82  O
HETATM 2387  O   HOH   159    13.208  60.522 -15.082  1.00  57.68  O
HETATM 2388  O   HOH   160    34.799  47.949 -14.048  1.00  71.55  O
HETATM 2389  O   HOH   161    12.156 -20.278  36.293  1.00  63.41  O
HETATM 2390  O   HOH   162    12.064   0.618  21.733  1.00  59.67  O
HETATM 2391  O   HOH   163    13.025  12.470  18.298  1.00  57.94  O
HETATM 2392  O   HOH   164    11.241  -6.036  37.279  1.00  66.37  O
HETATM 2393  O   HOH   165    15.326  30.761   7.083  1.00  72.54  O
HETATM 2394  O   HOH   166    24.166  26.288   8.146  1.00  80.46  O
HETATM 2395  O   HOH   167    18.532  37.307  28.877  1.00  52.52  O
HETATM 2396  O   HOH   169    19.929  10.591  15.027  1.00  79.89  O
HETATM 2397  O   HOH   171    18.161  19.995  12.208  1.00  88.12  O
HETATM 2398  O   HOH   172    25.181 -23.987  37.247  1.00  83.59  O
HETATM 2399  O   HOH   174    18.136  -3.696  37.260  1.00  58.69  O
HETATM 2400  O   HOH   175     9.790  35.898   8.924  1.00  68.04  O
HETATM 2401  O   HOH   176    39.649  55.783 -13.588  1.00  75.74  O
HETATM 2402  O   HOH   177    11.431 -13.326  32.112  1.00  68.92  O
HETATM 2403  O   HOH   178    15.462  13.080  15.436  1.00  72.04  O
HETATM 2404  O   HOH   179    10.845 -23.387  30.834  1.00  75.68  O
HETATM 2405  O   HOH   180     8.771  -8.704  37.430  1.00  69.36  O
HETATM 2406  O   HOH   181    21.236  41.306 -18.704  1.00  71.93  O
HETATM 2407  O   HOH   182    15.632  39.325  24.779  1.00  76.42  O
HETATM 2408  O   HOH   184     9.633   7.268  24.170  1.00  59.85  O
HETATM 2409  O   HOH   185     8.212  -4.659  26.095  1.00  73.13  O
HETATM 2410  O   HOH   187    22.544 -23.667  22.886  1.00  67.43  O
HETATM 2411  O   HOH   190    38.135  52.923 -18.866  1.00  60.86  O
HETATM 2412  O   HOH   192    13.987 -13.566  39.379  1.00  64.17  O
HETATM 2413  O   HOH   194     8.678  19.753  34.818  1.00  74.26  O
HETATM 2414  O   HOH   195    16.248  11.313  17.210  1.00  71.99  O
HETATM 2415  O   HOH   196    21.583  37.449 -18.466  1.00  74.25  O
HETATM 2416  O   HOH   197    18.608  13.183  13.886  1.00  69.55  O
HETATM 2417  O   HOH   199    32.100  47.030 -11.918  1.00  55.13  O
```

Figure 2 (Table 2 (page 51))

```
HETATM 2418  O    HOH    200      8.309  -2.904  23.865  1.00  78.50  O
HETATM 2419  O    HOH    201     27.690  42.102   3.955  1.00  77.78  O
HETATM 2420  O    HOH    204     13.069  56.872  -6.846  1.00  79.77  O
HETATM 2421  O    HOH    205     13.299   3.871  18.787  1.00  66.67  O
HETATM 2422  O    HOH    206     29.245  60.023 -30.224  1.00  60.72  O
HETATM 2423  O    HOH    208     14.879  -4.423  17.190  1.00  90.36  O
HETATM 2424  O    HOH    209     10.483  17.298  32.627  1.00  73.09  O
HETATM 2425  O    HOH    210     11.855  61.308 -30.434  1.00  88.84  O
HETATM 2426  O    HOH    211     13.217  40.439  25.017  1.00  85.86  O
HETATM 2427  O    HOH    213      7.822 -16.528  22.942  1.00  78.51  O
HETATM 2428  O    HOH    214     23.675  20.955  33.560  1.00  73.68  O
HETATM 2429  O    HOH    215      8.958 -13.070  31.871  1.00  66.49  O
HETATM 2430  O    HOH    216     13.965   9.052  16.630  1.00  67.53  O
HETATM 2431  O    HOH    220      8.596  -0.069  28.112  1.00  61.80  O
HETATM 2432  O    HOH    221     31.299  38.557 -18.341  1.00  61.93  O
HETATM 2433  O    HOH    222     20.516  15.336  17.249  1.00  62.41  O
HETATM 2434  O    HOH    223     32.487  45.347 -13.991  1.00  67.08  O
HETATM 2435  O    HOH    224      9.634  26.343  28.605  1.00  80.33  O
HETATM 2436  O    HOH    225     26.881  41.843   6.770  1.00  66.49  O
HETATM 2437  O    HOH    226     21.933  62.656  -9.449  1.00  77.20  O
HETATM 2438  O    HOH    227     16.939  -0.959  38.266  1.00  47.64  O
HETATM 2439  O    HOH    228      1.517  27.871  29.550  1.00  69.94  O
HETATM 2440  O    HOH    229     25.455  67.088 -17.467  1.00  70.28  O
HETATM 2441  O    HOH    231     22.761  36.354 -14.024  1.00  67.12  O
HETATM 2442  O    HOH    233      9.742 -18.263  29.864  1.00  71.11  O
HETATM 2443  O    HOH    236      9.749  -1.644  39.210  1.00  68.73  O
HETATM 2444  O    HOH    238     18.795  37.370  -0.374  1.00  70.06  O
HETATM 2445  O    HOH    239     28.893 -23.822  27.314  1.00  63.21  O
HETATM 2446  O    HOH    240     20.653  54.689  -2.794  1.00  69.17  O
HETATM 2447  O    HOH    241     32.703  57.255  -7.932  1.00  73.68  O
HETATM 2448  O    HOH    242     26.839  45.754 -28.862  1.00  73.66  O
HETATM 2449  O    HOH    243     21.145  36.229  -1.718  1.00  67.47  O
HETATM 2450  O    HOH    244     24.749  63.978 -31.459  1.00  70.06  O
HETATM 2451  O    HOH    245     15.031  42.223  -0.424  1.00  65.72  O
HETATM 2452  O    HOH    246     13.421  46.493   5.518  1.00  68.84  O
HETATM 2453  O    HOH    247     31.086  37.829 -20.633  1.00  67.16  O
HETATM 2454  O    HOH    249     16.331  24.733   8.656  1.00  80.75  O
HETATM 2455  O    HOH    250     34.686  48.482 -11.577  1.00  67.41  O
HETATM 2456  O    HOH    252     26.863 -21.667  27.711  1.00  73.87  O
HETATM 2457  O    HOH    253     25.486  24.675   5.799  1.00  94.36  O
HETATM 2458  O    HOH    255     19.570 -18.069  15.539  1.00  68.87  O
HETATM 2459  O    HOH    256      7.507  24.181  27.128  1.00  75.95  O
HETATM 2460  O    HOH    257     18.214  50.275  13.595  1.00  77.43  O
HETATM 2461  O    HOH    258     24.259   5.598  21.754  1.00  80.04  O
HETATM 2462  O    HOH    259     23.644  -9.401  38.458  1.00  73.87  O
HETATM 2463  O    HOH    260     29.288  57.908 -36.191  1.00  83.70  O
HETATM 2464  O    HOH    261     14.644 -13.020  15.667  1.00  67.62  O
HETATM 2465  O    HOH    262     16.016  47.827  16.745  1.00  77.21  O
HETATM 2466  O    HOH    263     19.538 -33.347  29.648  1.00  64.40  O
HETATM 2467  O    HOH    265      2.949  33.426  13.572  1.00  75.54  O
HETATM 2468  O    HOH    266     25.030  51.698 -23.955  1.00  72.53  O
HETATM 2469  O    HOH    267     29.126  34.667  -5.967  1.00  87.07  O
HETATM 2470  O    HOH    268     21.351   0.866  18.679  1.00  81.24  O
HETATM 2471  O    HOH    270     11.563 -28.282  33.256  1.00  88.99  O
HETATM 2472  O    HOH    273     25.953  36.560 -14.131  1.00  68.45  O
HETATM 2473  O    HOH    275      3.498  32.668  11.344  1.00  60.17  O
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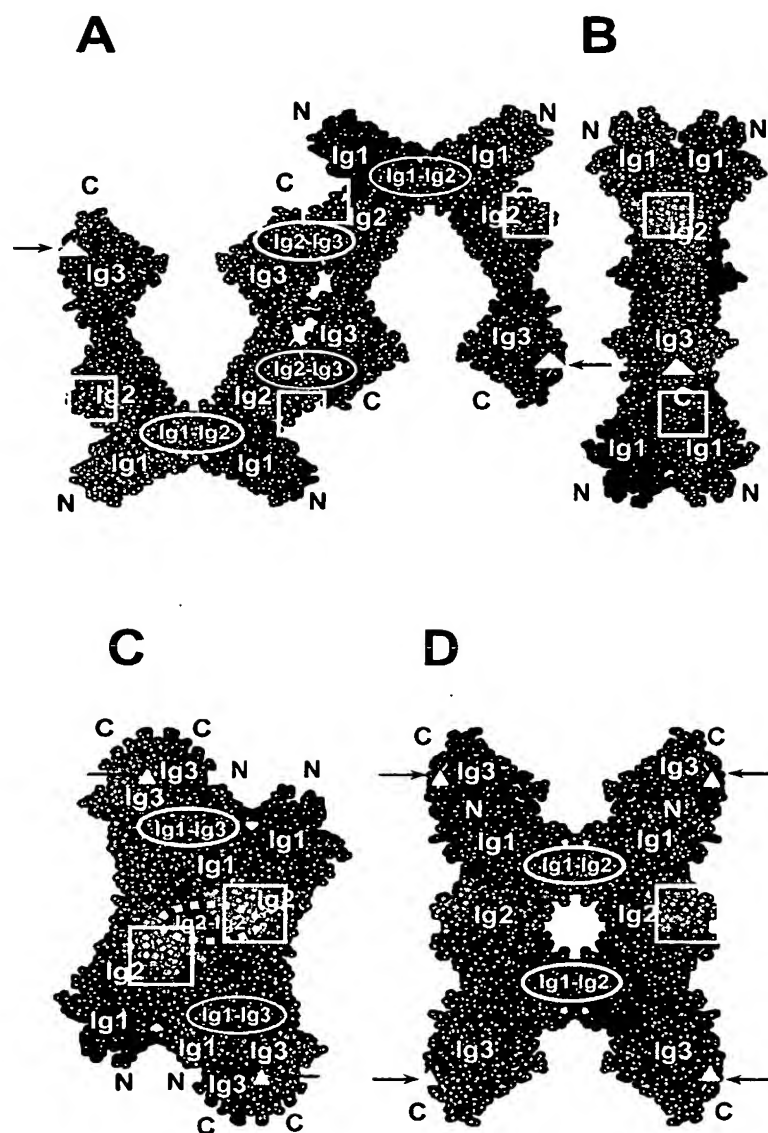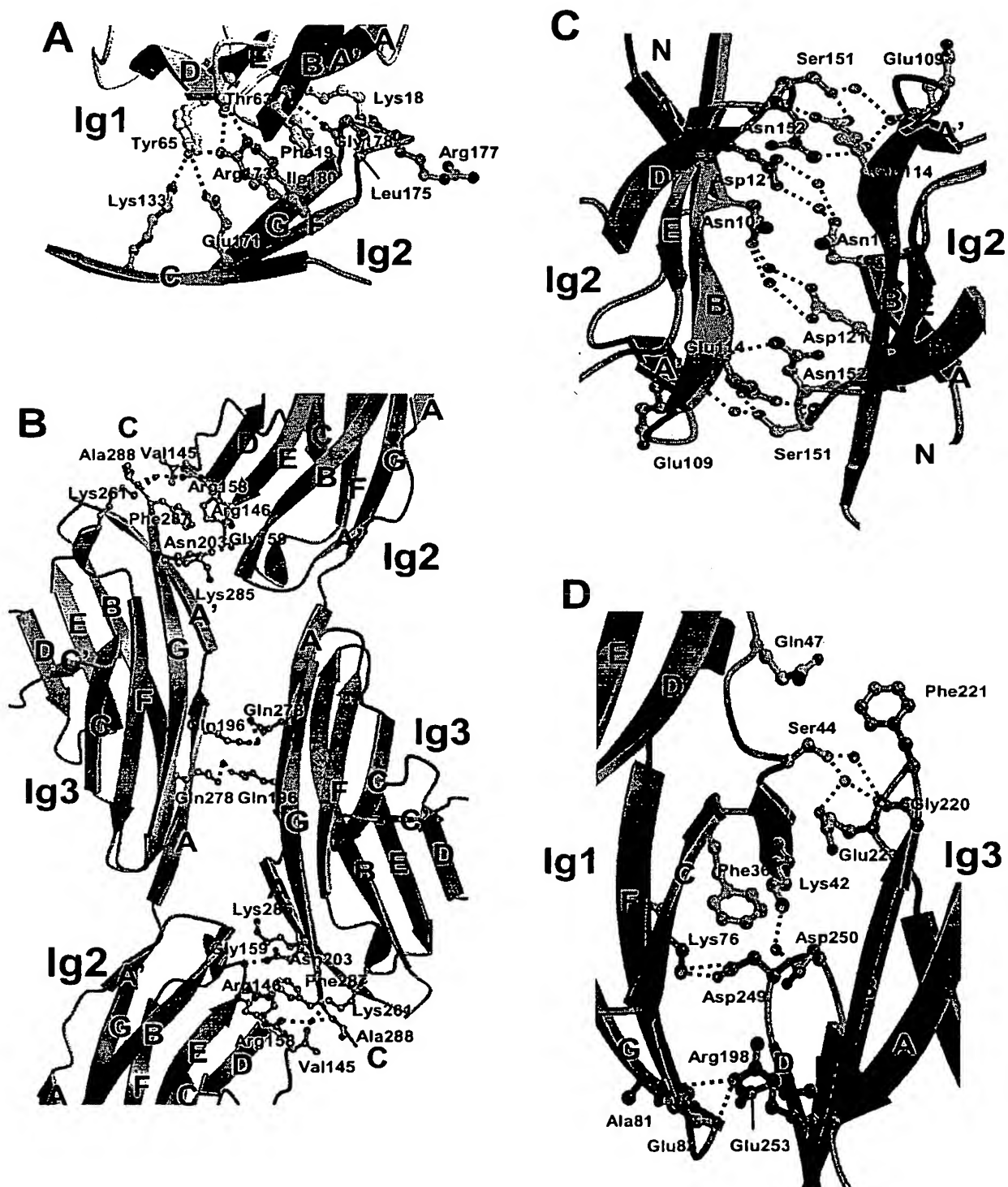
Figure 2 (Table 2 (page 52))

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HETATM 2474   O   HOH   277      24.261 -20.185  20.738  1.00 69.47 O
HETATM 2475   O   HOH   279      16.935  12.111  32.241  1.00 61.50 O
HETATM 2476   O   HOH   281       6.985  31.018  33.495  1.00 82.04 O
HETATM 2477   O   HOH   282      29.259  66.155 -18.386  1.00 76.82 O
HETATM 2478   O   HOH   283       7.960  15.959  16.209  1.00 82.31 O
HETATM 2479   O   HOH   284      10.497 -27.436  17.219  1.00 87.04 O
HETATM 2480   O   HOH   286      26.964  63.396 -39.492  1.00 92.90 O
HETATM 2481   O   HOH   288      24.134  68.136 -30.170  1.00 73.68 O
HETATM 2482   O   HOH   289      21.035  57.596  -2.427  1.00 63.71 O
HETATM 2483   O   HOH   290       5.098  -6.663   9.498  1.00 71.30 O
HETATM 2484   O   HOH   291      28.355  60.022 -32.628  1.00 84.14 O
HETATM 2485   O   HOH   292      27.829 -18.993  32.106  1.00 83.61 O
HETATM 2486   O   HOH   294      25.765  53.781 -27.581  1.00 80.50 O
HETATM 2487   O   HOH   295      24.969 -15.013  17.181  1.00 79.45 O
HETATM 2488   O   HOH   296      21.804 -31.840  29.638  1.00 63.37 O
HETATM 2489   O   HOH   297      24.675  41.475  22.470  1.00 76.81 O
HETATM 2490   O   HOH   298      21.097 -16.469  16.858  1.00 76.40 O
HETATM 2491   O   HOH   299      10.492   1.947  39.785  1.00 73.55 O
HETATM 2492   O   HOH   300      24.883  60.577  -6.394  1.00 83.17 O
HETATM 2493   O   HOH   301      12.022  63.003 -25.379  1.00 82.86 O
HETATM 2494   O   HOH   302      29.658  36.500 -13.658  1.00 76.81 O
HETATM 2495   O   HOH   303      28.183  35.860 -10.762  1.00 71.74 O
HETATM 2496   O   HOH   304      33.215  39.854  -9.262  1.00 79.17 O
HETATM 2497   O   HOH   305      22.138  35.777 -10.127  1.00 75.26 O
HETATM 2498   O   HOH   306      34.862  51.476  -6.285  1.00 73.10 O
HETATM 2499   O   HOH   307      40.147  51.580  -7.567  1.00 79.78 O
HETATM 2500   O   HOH   308      28.423  71.917 -29.800  1.00 75.06 O
HETATM 2501   O   HOH   309      31.298  68.573 -22.781  1.00 78.92 O
HETATM 2502   O   HOH   310      22.252  33.788   4.586  1.00 75.58 O
HETATM 2503   O   HOH   311      26.312  13.773  26.214  1.00 71.75 O
HETATM 2504   O   HOH   312      24.723  12.029  25.114  1.00 75.67 O
HETATM 2505   O   HOH   313      23.485  49.266   5.646  1.00 72.55 O
HETATM 2506   O   HOH   314      25.648  43.055  12.920  1.00 71.36 O
HETATM 2507   O   HOH   315       4.653  34.503  32.710  1.00 77.71 O
HETATM 2508   O   HOH   316       2.456  37.131  32.175  1.00 78.77 O
HETATM 2509   O   HOH   317       6.881  27.100  34.488  1.00 80.24 O
HETATM 2510   O   HOH   318      10.082  23.711  13.099  1.00 81.07 O
HETATM 2511   O   HOH   319      18.524 -28.499  21.428  1.00 79.53 O
HETATM 2512   O   HOH   321      26.684   3.017  30.716  1.00 82.34 O
HETATM 2513   O   HOH   322      27.178  -5.228  32.903  1.00 82.07 O
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CONECT  603  174
CONECT  932 1341
CONECT 1341  932
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CONECT 2094 1686
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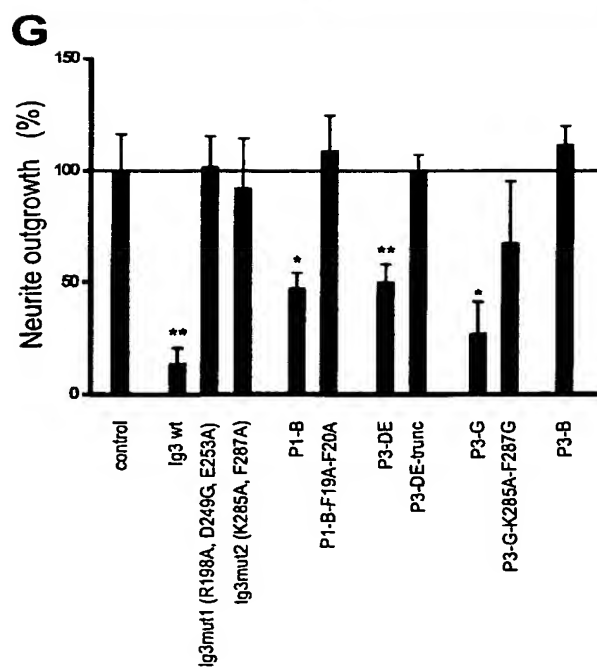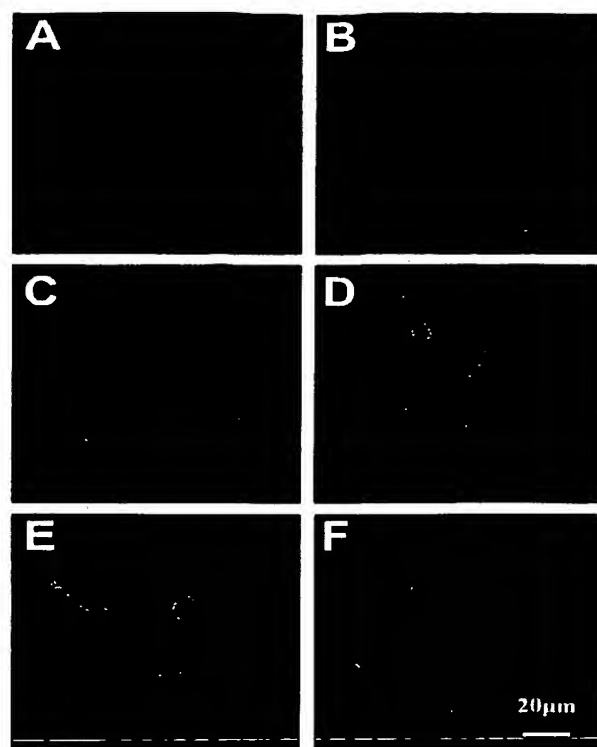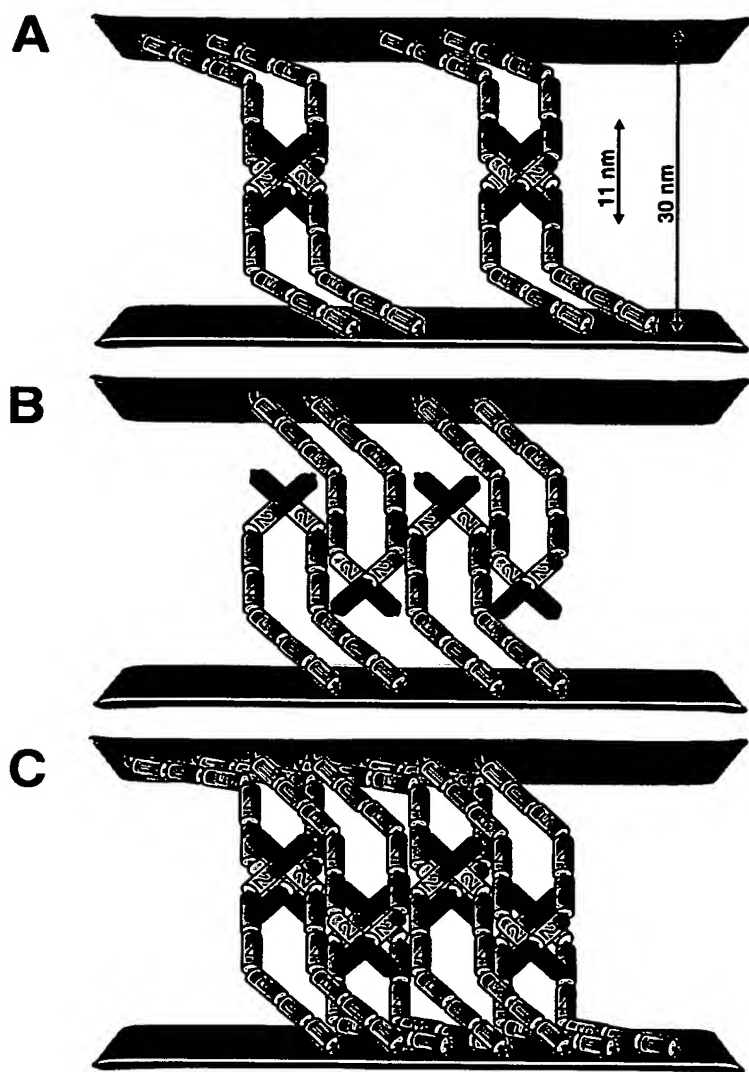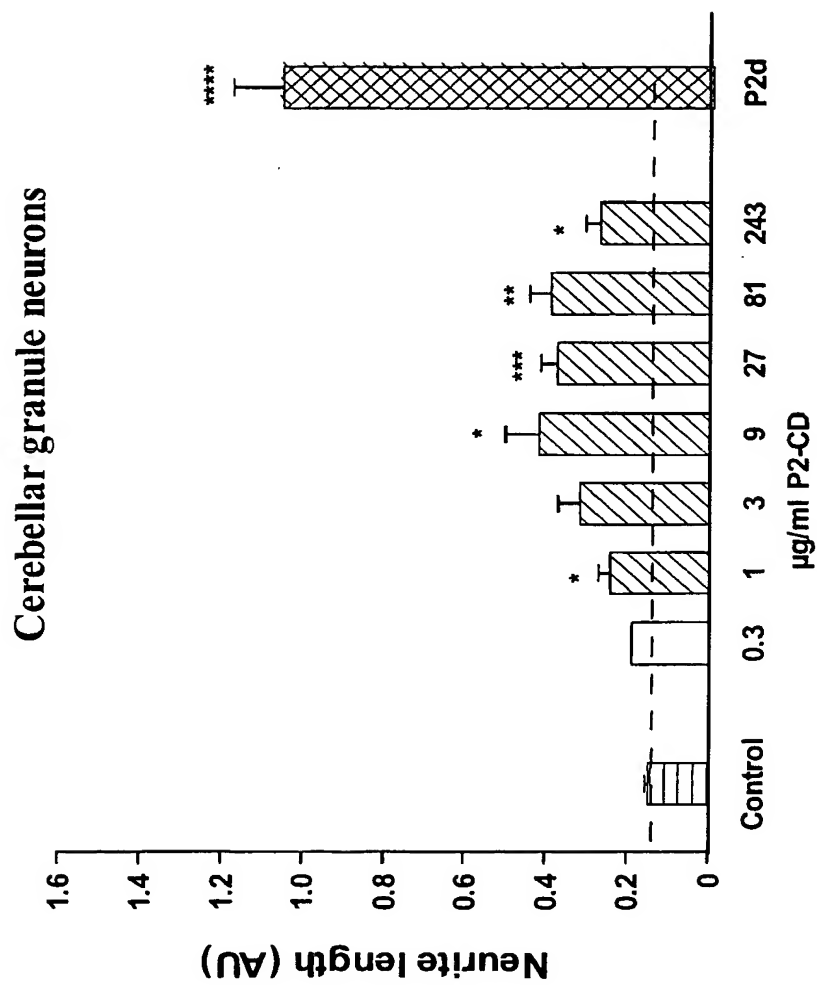
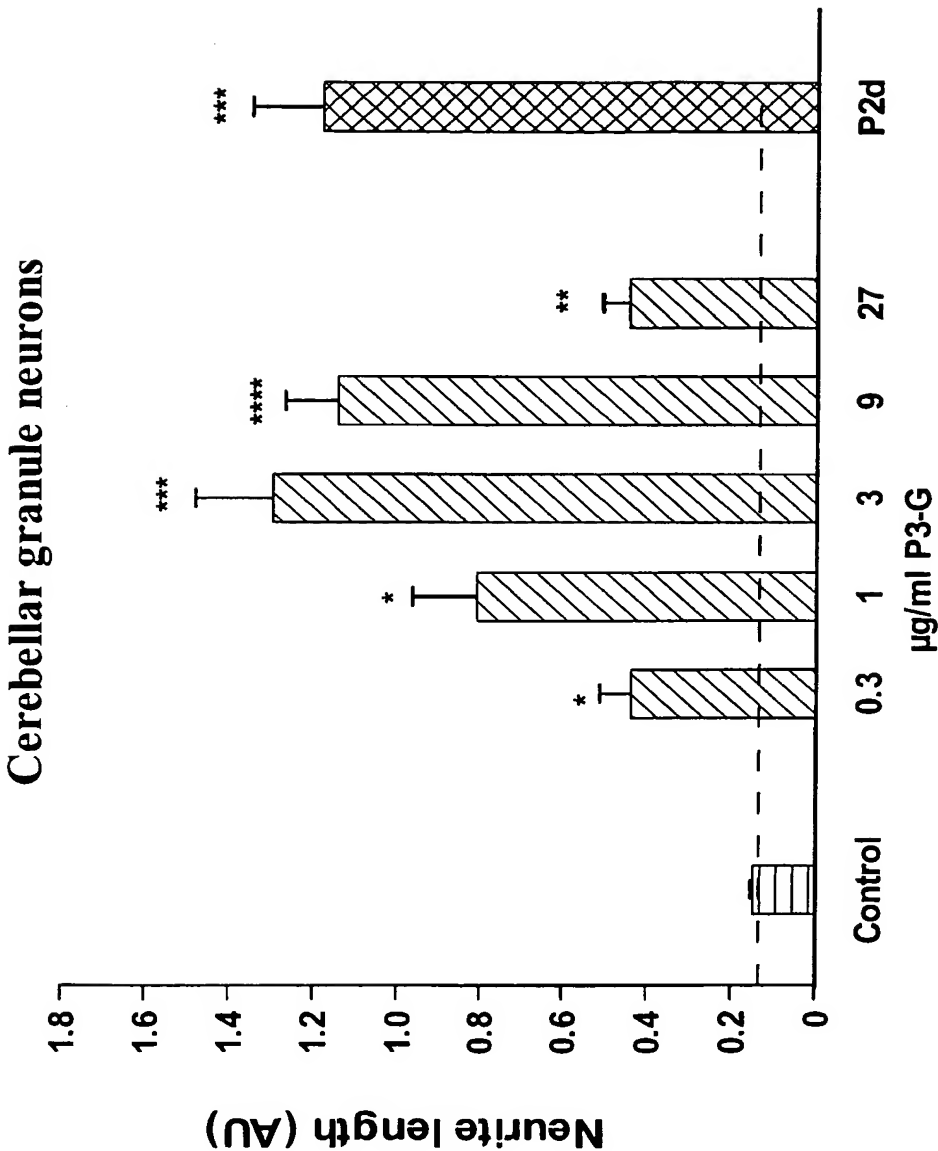**Figure 3**

Figure 4

Figure 5
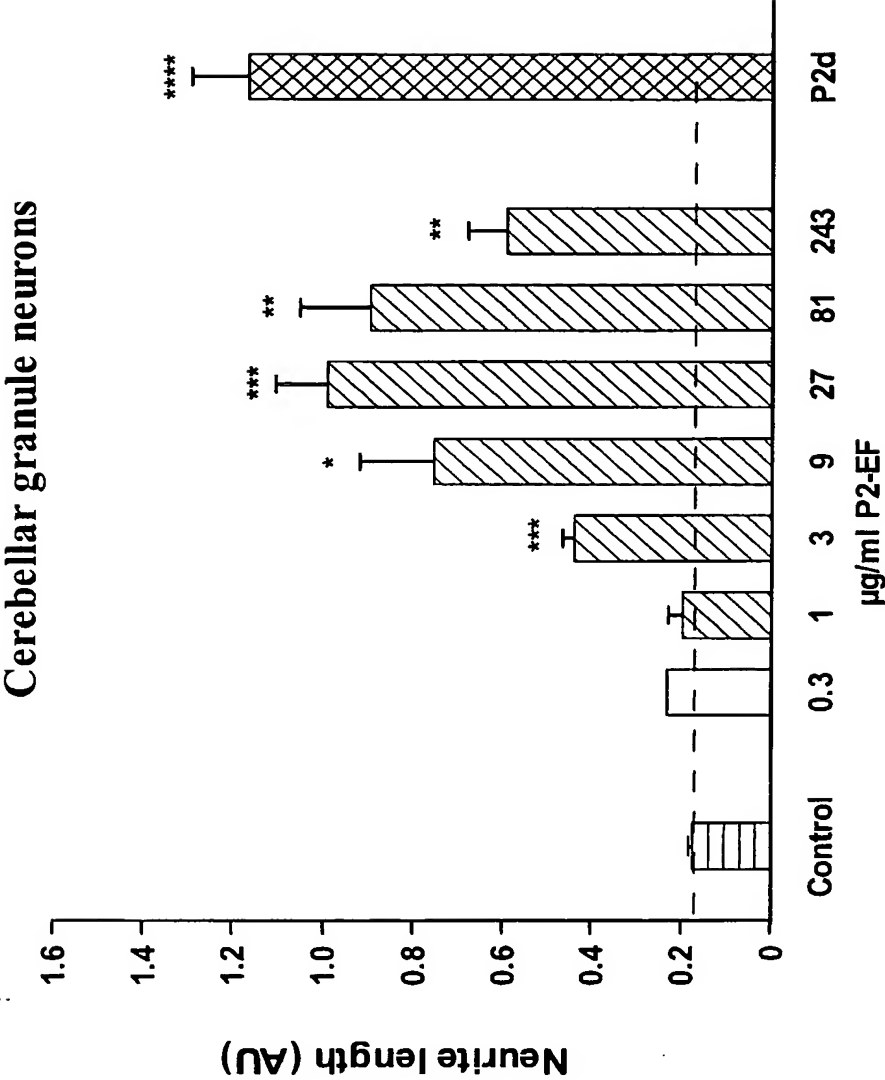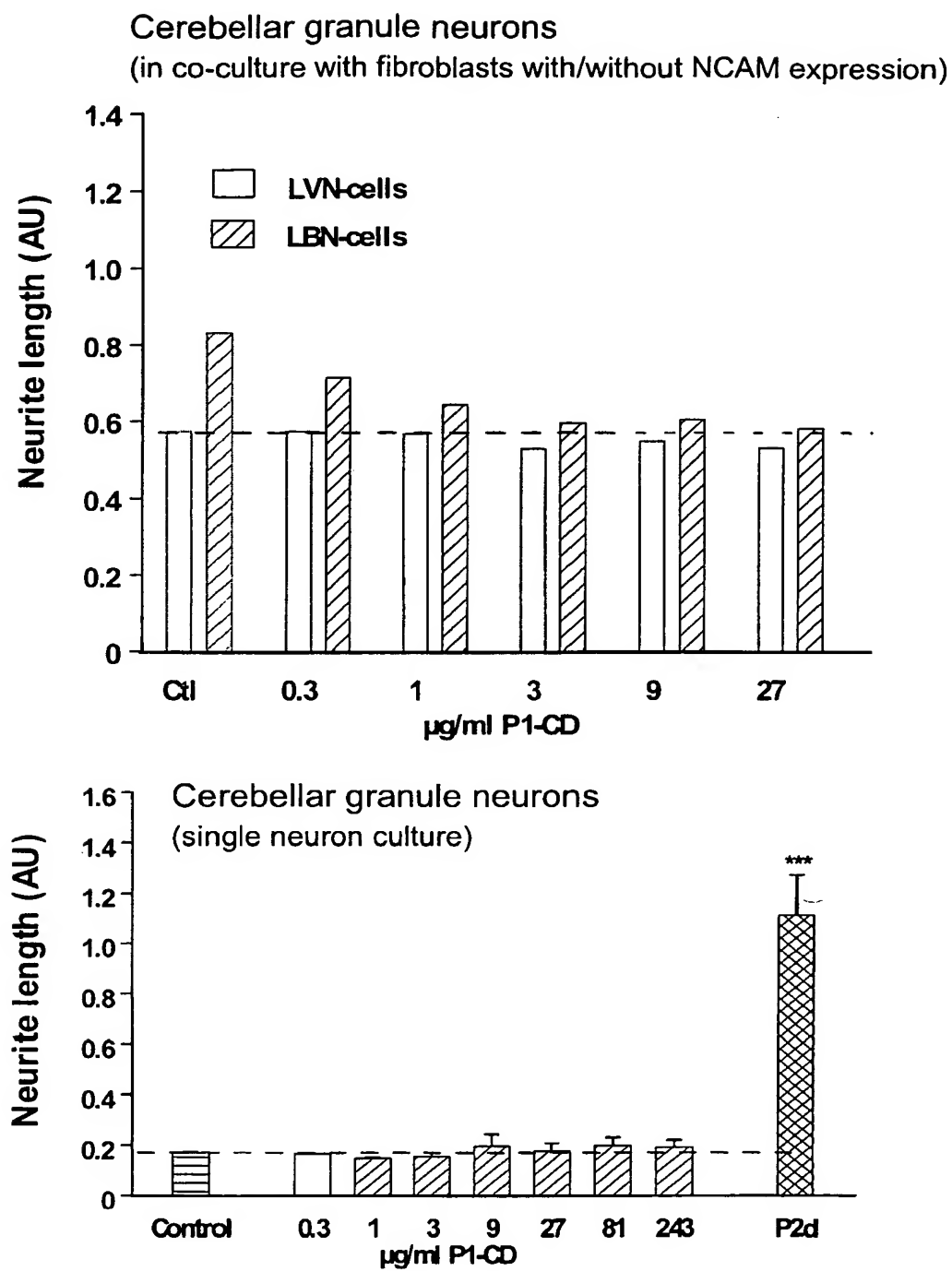
Figure 6

Figure 7

Figure 8

Figure 9

Figure 10

Cerebellar granule neurons
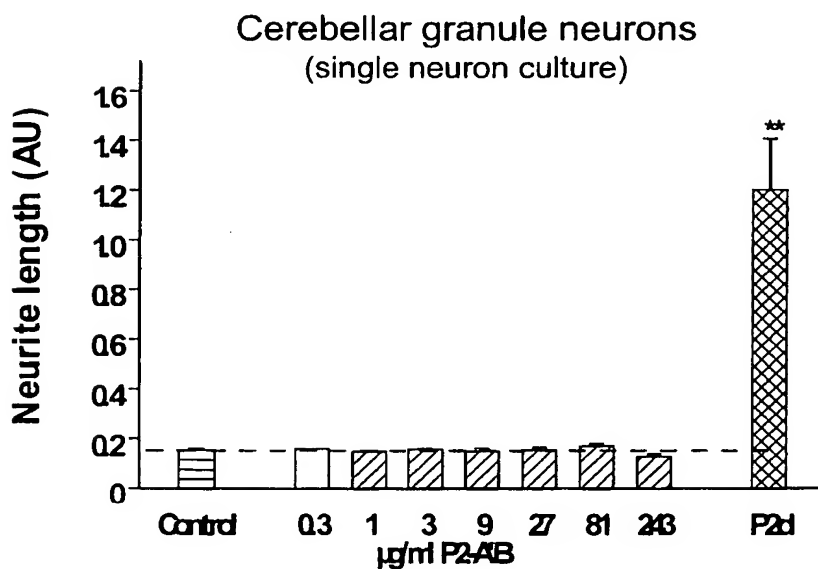(in co-culture with fibroblasts with/without NCAM expression)

Cerebellar granule neurons
(single neuron culture)

Figure 11

Cerebellar granule neurons
(in co-culture with fibroblasts with(without NCAM expression)
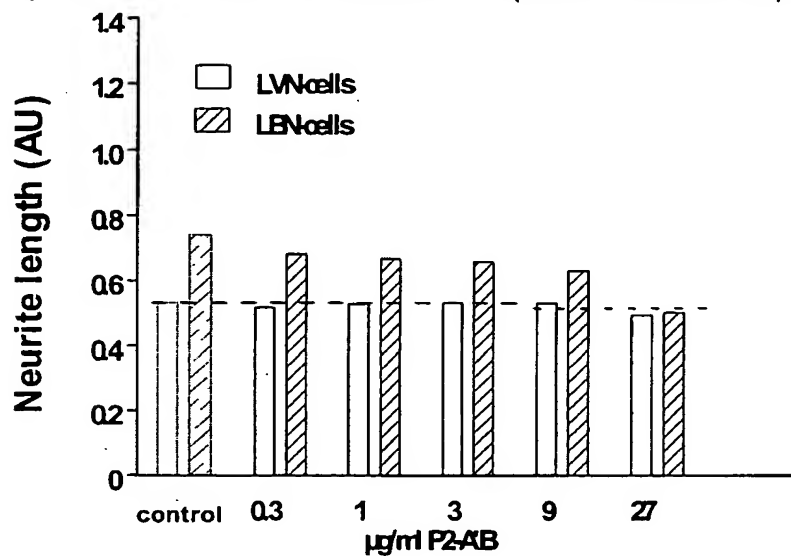
Cerebellar granule neurons
(single neuron culture)

Figure 12